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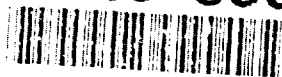||||||||||||||||||||||

HYDROGEOLOGIC EFFECTS
OF IN-SITU GROUNDWATER TREATMENT
USING BIODEGRADATION

by

Grant Garven, Principal Investigator
Werner Siebert, Graduate Student

Department of Earth and Planetary Sciences
The Johns Hopkins University
Baltimore, Maryland 21218

for

U.S. Army Toxic and Hazardous Materials Agency
Aberdeen Proving Ground (Edgewood Area), Maryland 21010

June 15, 1987

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No 0704-0188
Exp Date Jun 30, 1986

1a. REPORT SECURITY CLASSIFICATION	1b. RESTRICTIVE MARKINGS
UNCLASSIFIED	
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	Distribution Unlimited.
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S)
Delivery Order 2378	TCN 86-242

6a. NAME OF PERFORMING ORGANIZATION	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION
The Johns Hopkins University		U.S. Army Research Office
6c. ADDRESS (City, State, and ZIP Code)		7b. ADDRESS (City, State, and ZIP Code)
Attn: Grant Garven Dept. of Earth & Planetary Sciences Baltimore, MD 21218		P.O. Box 12211 Research Triangle Park, NC 27709-2211

8a. NAME OF FUNDING/SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
US Army THAMA	AMXTH-TE-D	

8c. ADDRESS (City, State, and ZIP Code) (J. L. Mahannah)	10. SOURCE OF FUNDING NUMBERS			
Aberdeen Proving Ground, MD 21010-5401	PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO

11. TITLE (Include Security Classification)

IN-SITU GROUNDWATER TREATMENT

12. PERSONAL AUTHOR(S)   Grant Garven

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
FINAL REPORT	FROM 5/27/86 TO 5/26/87	June 15, 1987	

16. SUPPLEMENTARY NOTATION   Task was performed under a Scientific Services Agreement issued by Battelle, Research Triangle Park Office, 200 Park Drive, P.O. Box 12297, Research Triangle Park, NC 27709

17.	COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	HYDROGEOLOGIC EFFECTS BIODEGRADATION
			GROUNDWATER TREATMENT

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Several in-situ biorestoration scenarios are described in the report, mostly with application to contamination in extensive sand aquifers. Evaluation of the various methods, however, is likely to be site specific, given the complexities of most geologic settings and groundwater systems. The application of in-situ schemes for clayey deposits or fractured rock are unknown. A major finding from this research is the potential effect of biofouling on the site hydrology. Permeability, for example, can be reduced by several orders of magnitude due to microbial growth in granular porous media. Laboratory benchtop experiments confirmed the permeability reduction at a macroscopic scale. Mathematical models are presented also to demonstrate the possible effect at the aquifer scale, but only site-specific pilot studies can confirm these results.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☐ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	
22a. NAME OF RESPONSIBLE INDIVIDUAL JANET L. MAHANNAH	22b. TELEPHONE (Include Area Code) (301) 671-2054 22c. OFFICE SYMBOL AMXTH-TE-D

DD FORM 1473, 84 MAR   83 APR edition may be used until exhausted.   SECURITY CLASSIFICATION OF THIS PAGE
All other editions are obsolete.

UNCLASSIFIED

EXECUTIVE SUMMARY

Subsurface contamination by organic compounds has become a major environmental problem at various U.S.Army installations. The technology exists to experiment with biological in-situ degradation methods of treatment and reclamation, but the factors controlling the chemical and physical environments of biodegradation are not well known and few site-specific case studies are documented in the engineering literature. The purpose of this study was to identify applicable in-situ groundwater treatment methods and performance criteria, and to help evaluate these techniques, especially with respect to limitations imposed by hydrogeologic conditions.

Several in-situ biorestoration scenarios are described in the report, mostly with application to contamination in extensive sand aquifers. Evaluation of the various methods, however, is likely to be site specific, given the complexities of most geologic settings and groundwater systems. The application of in-situ schemes for clayey deposits or fractured rock are unknown. A major finding from this research is the potential effect of biofouling on the site hydrology. Permeability, for example, can be reduced by several orders of magnitude due to microbial growth in granular porous media. Laboratory benchtop experiments confirmed the permeability reduction at a macroscopic scale. Mathematical models are presented also to demonstrate the possible effect at the aquifer scale, but only site-specific pilot studies can confirm these results.

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1. Introduction

Subsurface contamination of groundwater by organic compounds has become a major environmental problem at various U.S. Army installations throughout the country. It is essential to find appropriate reclamation methods to limit and reduce the extent of contamination. Restoration of polluted aquifers by means of biological in-situ methods, which use microorganisms to degrade toxic organic contaminants, has recently been applied with some success and has been shown to be cost-effective (Wilson et al., 1985, Wagner et al.,1986). These in-situ methods will herein be referred to in this text as bioreclamation or biorestoration. The basic method of bioreclamation is to enhance bacterial growth in the subsurface by the injection of bionutrients. Heterotrophic bacteria can use toxic organic compounds as a source of carbon as well as a source of energy, thereby degrading and detoxifying the contaminants. The mechanism of these biorestoration methods, however, is still under research and little is known about the biochemical interactions during biodegradation processes (Pinder and Gray, 1984, Wilson et al., 1985).

A further unknown factor, which will be critical in actual field installations, is the physical effect of microbial growth on the hydraulic properties of porous media. The permeability of a sand aquifer, for example, can be altered by orders of magnitude due to microbial growth. This type of clogging effect would have a substantial influence on the transport of contaminants in groundwater and therefore on the design of restoration schemes.

2. Objectives of Research

In this research we have tried to quantify the changes in hydraulic parameters due to microbial activity and to outline the importance of these changes for the reclamation design and evaluation of performance criteria. Our method of analysis

included:

- A literature review to identify possible in-situ reclamation schemes.

- Collection of data from laboratory permeameter experiments to determine changes in permeability under a variety of controlled conditions.

- Development of a hydrogeologic simulation model capable of mathematically modeling two-dimensional mass transport in groundwater flow and incorporating the effects of biological processes on permeability to assess the importance of these effects for bioreclamation designs.

The goal of this research will be eventually to apply the experimental data and the numerical model to hydrogeologic settings typical of site conditions at U.S.Army installations for the development of simulations of aquifer restoration in order to evaluate the reclamation procedure and its effects on hydraulics of the groundwater system.

3. Bioreclamation

Treatment Methods

There are a wide range of possible treatment methods available to reclamate contaminated groundwater. The conventional methods are:

- elimination of the contaminant source by excavating it and depositing it at hazardous waste disposal sites,

- isolating the contaminant source by surrounding it with low permeability slurry walls, or through the development of groundwater divides,

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- removal of contaminated water through pumping followed by above ground treatment,

Excavating the contaminant source is not always an economically feasible method. The excavation costs are high and workers and the environment have to be protected against the hazardous chemicals being exposed during excavation. The problem sometimes is not resolved by depositing the contaminant at a hazardous waste disposal site. The construction of low permeability slurry walls can be cost-extensive (Zipfel and Geldner, 1985), but isolating the contaminant does not eliminate it. There exists also the possibility that certain chemicals could attack the slurry walls and render them more permeable. Thus, a continuous monitoring system becomes neccessary. Removal of contaminated water through well pumping is also cost-effective for small spills, but this becomes impractical or too expensive for large contaminant plumes in aquifers.

In-situ hydraulic methods are often used in connection with chemical or biological in-situ techniques. If they are applicable and prove to be successful, these in-situ techniques would have the advantage to eliminate the contamination at place. The site would need to be monitored only for the limited time of treatment. The hazardous chemical is left in the ground and does therefore not present a health threat to workers. The aquifer can be used again after successful reclamation (Nagel et al., 1982). Among the in-situ methods bioreclamation methods seem to show the most promise (Wagner et al., 1986).

Bioreclamation

The principle of bioreclamation is based on the biodegradability of the organic contaminant. Bacterial growth is enhanced at the location of the contaminants by injecting nutrients and oxygen. Figure 1 shows a possible scenario of a bioreclamation. The nutrient water is either injected by a well or infiltrated. Oxygen can be

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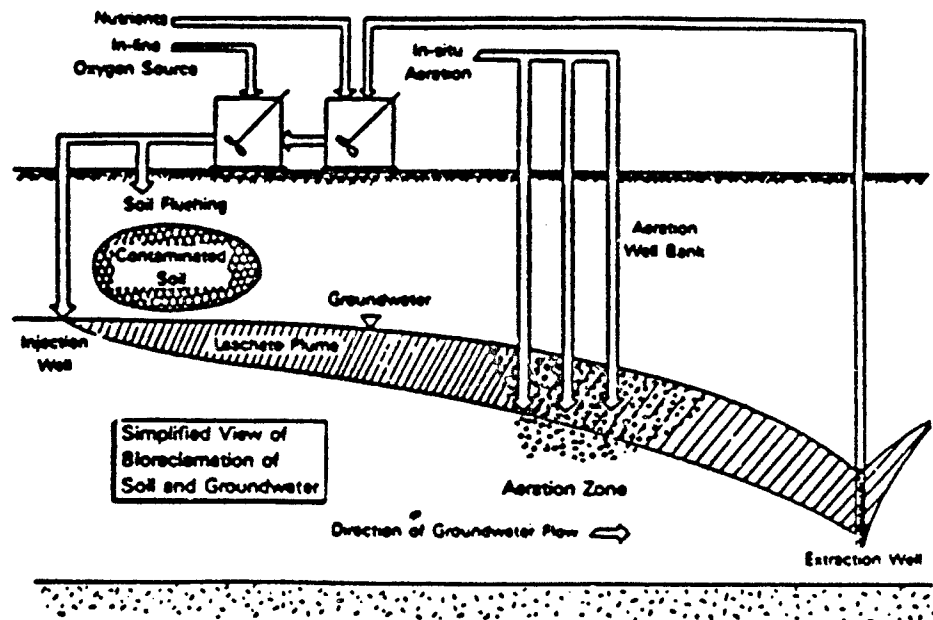
Figure 1: Conceptual model for in situ biorestoration. Nutrients can either be injected by wells or infiltrated through flooding or spray irrigation. Oxygen can either be added in line to the nutrient solution or directly injected into the contaminated area through aeration wells. (from Wagner et al., 1986)

added in-line or directly injected by aeration wells into the contaminant plume.

Conditions for Biodegradation

Numerous researchers have shown in laboratory experiments (Alexander, 1981; Kobayashi, 1982; Bouwer, 1984) that hazardous organic contaminants are actually transformed by bacteria into non-toxic compounds. Most compounds are degraded aerobically whereas lower-molecular weight halogenated-hydrocarbons degrade only anaerobically (Bouwer, 1981; Wagner et al., 1986). The potential for utilizing biodegradation in the subsurface also exists because of recent work showing the presence of bacteria (Sykes et al., 1982; Schwarzenbach et al., 1983; Wilson et al., 1983). Bacteria adapted to the contaminant in the laboratory can be introduced into the aquifer but in most bioreclamation cases bacteria indigenous to the aquifer are used.

Nutrients must be added to the aquifer in order to enhance bacterial activity. The composition of these nutrients can be tailored for existing geochemical and biological conditions. In some cases, when the contaminant is either toxic to bacteria or its concentration is too low, bacterial growth cannot be supported by the organic contaminant alone. Another carbon source such as glucose or citrate has to be provided as a primary substrate to encourage bacterial growth (Wagner et al., 1986).

Sufficient oxygen supply is crucial for aerobic degradation, where oxygen serves as electron acceptor. The injection of air into the groundwater has limited application for contaminations of low concentration, because of the relative low solubility of oxygen in water. This difficulty is overcome by the use of pure oxygen and hydrogen peroxide. Hydrogen peroxide has the additional advantage of reducing clogging around injection wells due to its relative toxicity to bacteria, and it decomposes quickly into water and oxygen thus reducing its toxicity and making oxygen available to the bacteria.

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Design of Bioreclamation Systems

Nutrients and oxygen have to be injected or transported into the contamination site. Injection and extraction systems are the two basic units of a biorestoration scheme. The transport of nutrients and oxygen can be gravity driven or forced by pumping wells. If the soil is permeable enough to allow percolation the nutrient water can be applied to the contamination site by spray irrigation or flooding. In less permeable soils subsurface drains might be appropriate (Figure 2). The application of subsurface drains is, however, limited to shallow contaminant plumes in unconsolidated media because the installation of the drainage system to greater depths could be too cost-intensive (Wagner, 1986). A wide variety of arrangements of injection and extraction wells are possible. In general, rows of wells injecting nutrients and oxygen are arranged upstream of the contamination plume. Extraction wells are located downstream of the contamination site to collect the water. The water can be further treated aboveground and recharged into the aquifer through the injection wells after addition of nutrients and/or oxygen. Another group of wells, which inject fresh groundwater and are located around the wells injecting the recharged water with nutrients, create a hydraulic mound that prevents further contamination of the aquifer by recharge water (Figure 3). Additional recharge wells arranged along the contamination plume could optimize nutrient and oxygen supply to the contaminated area (Figure 4). If the groundwater flow direction and the extent of the plume is well known, a row of injection wells perpendicular to the groundwater flow direction infiltrating nutrients and oxygen, can eventually intercept the spread of the contamination (Figure 5). In all cases monitoring wells have to control the spatial extent of the contamination to make sure that the operational system is working efficiently and that the contamination plume is not spreading further.

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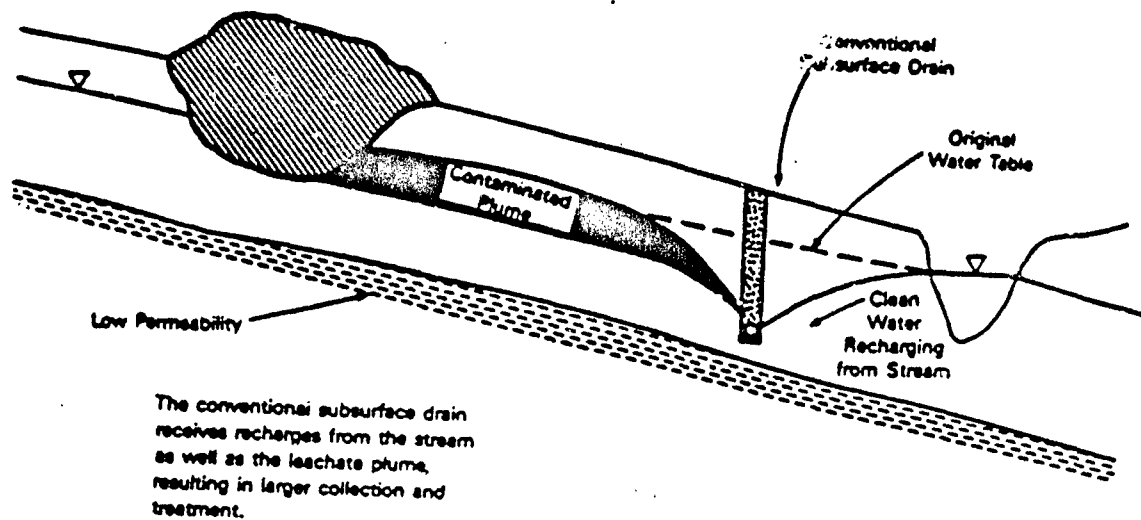
Figure 2: Bioreclamation with a subsurface drain. In less permeable soils a sub-surface drain may be more appropriate than extraction wells. (from Wagner et al., 1986)

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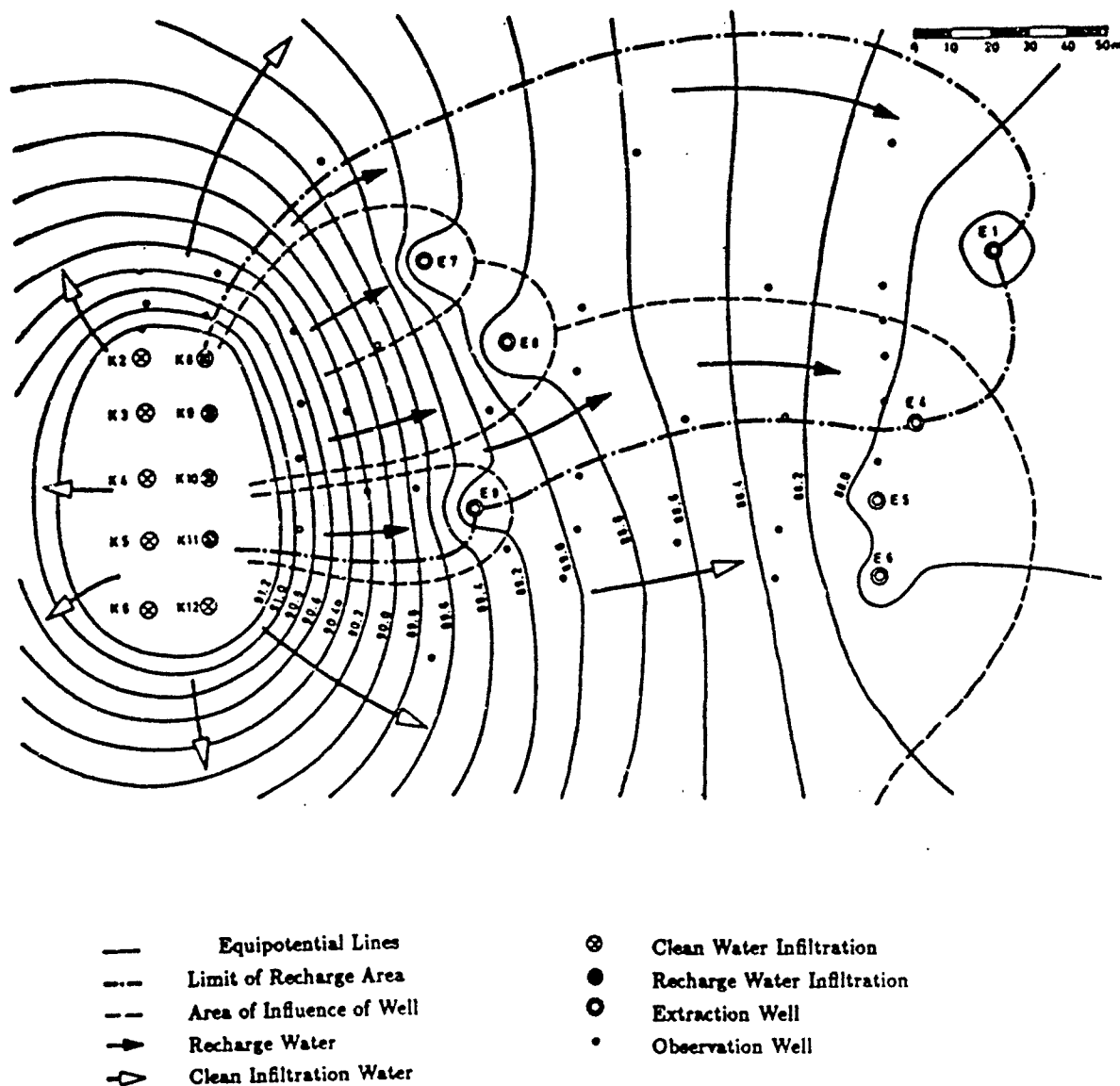
Figure 3: Bioreclamation with fresh water infiltration. During in-situ bioreclamation the polluted extracted groundwater is often treated, and after addition of nutrients and oxygen, recharged into the subsurface. Wells around the recharge wells, inject clean groundwater to prevent a contamination of the aquifer with the polluted recharge water. (after Battermann and Werner, 1984)
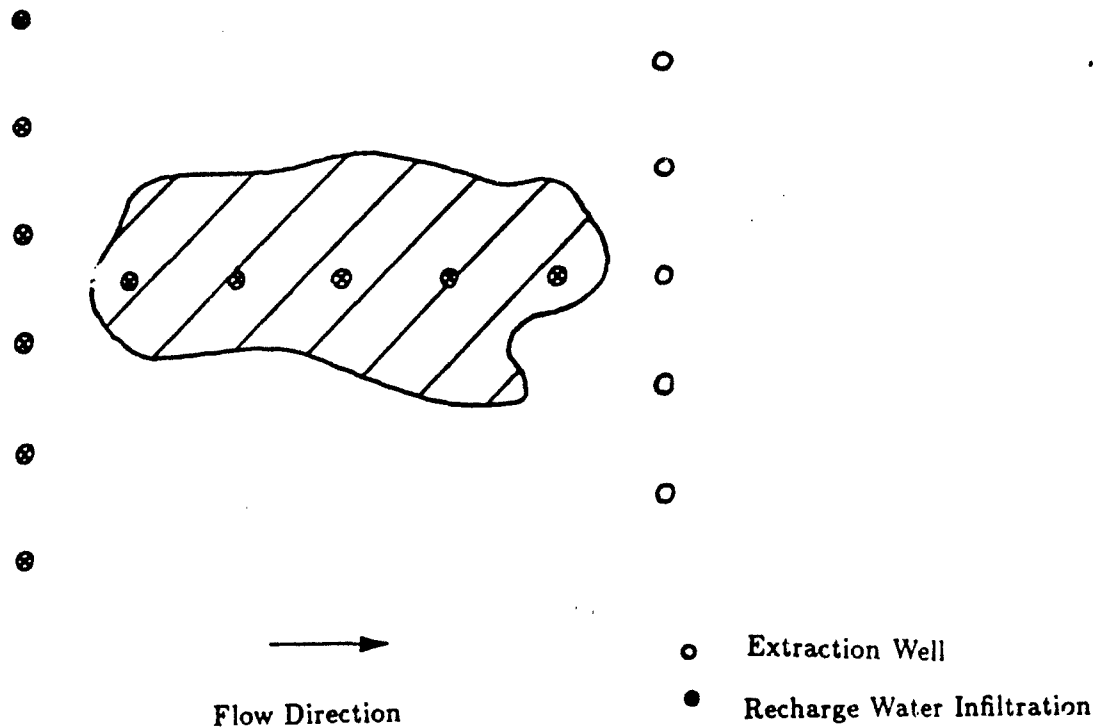
Figure 4: Bioreclamation with additional injection wells. This figure shows a possible configuration of injection and extraction wells suggested by Valocchi and Rittmann (1986). Injection wells along the contaminated plume would facilitate transport of nutrients and enhance biodegradation.

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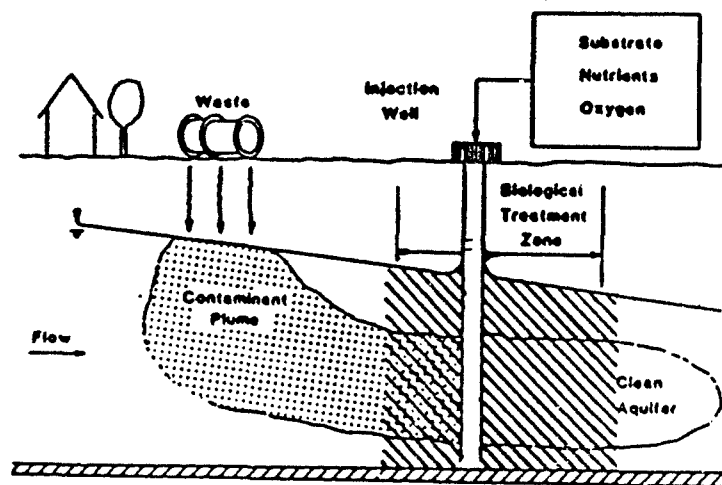
Figure 5: Bioreclamation with injection wells downstream from the contaminant source. A possible configuration scheme for a bioreclamation is to intercept the spread of a contaminant plume through injection wells downstream from the contaminant source. (after Bouwer, 1984)

4. Performance Criteria

The following performance criteria for the successful implementation of a bioreclamation were identified:

- previous experiences

- operation and monitoring requirements

- costs

- biodegradability

- bacterial contamination

- hydrogeological implications

Experiences from previous bioreclamation applications show that many organic contaminants can be biodegraded to concentrations below detection level (Nagel, 1982; Jhaveri, 1983). Bioreclamation has been applied only to spill sites so far, but since there is evidence of adapted bacterial communities below waste disposal sites, Wagner et al.(1986) suggest that bioreclamation methods are applicable to such cases as well. Depending on the duration of the bioreclamation system, operation and maintenance requirements can be quite expensive. A series of biochemical parameters such as pH, dissolved oxygen, concentration of contaminant, bacterial numbers, etc., have to be monitored constantly in order to maintain the efficiency of the reclamation process. These parameters can be corrected by addition of appropriate nutrients, oxygen, or by incubation of bacteria. In many bioreclamation cases, clogged wells had to be treated. The use of hydrogen peroxide has shown to be an effective agent for treating clogging effects (Yaniga, 1984). Estimations for operational and permanent costs are difficult to generalize because of the site-specific

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characteristics of a contamination site. It is also difficult to make any generalizations about costs since the success of a bioreclamation method is dependant on so many different parameters. Wagner et al.(1986) gives one example of a contamination site where the in-situ treatment of the contaminated groundwater through bioreclamation was an order of magnitude less costly than the above ground treatment of the polluted groundwater. Laboratory experiments have to prove that the organic contaminant is biodegradable by the bacterial population present. In some cases, a high heavy metal concentration could be toxic to bacteria and prevent successful biodegradation. The possibility also exist for contaminants to be transformed by bacteria into still more toxic compounds (Alexander, 1981). The rate of degradation depends on the characteristics of the organic contaminant and the bacterial population. If the degradation requires a long time, say 5-6 years, to occur, then due to high operational costs the expenses for bioreclamation might exceed those of a more conventional water treatment method. In other cases there exists concern about bacterial contamination. Little is known about the transport of bacteria in aquifers. Some tracer studies with viruses indicate that microorganisms can travel hundreds of meters (McDowell-Boyer et al., 1986). The proximity of water supply wells could raise concern about bioreclamation methods where bacterial growth is enhanced. In addition to these restrictions the success of a bioreclamation scheme will depend very strongly on the hydrogeological situation of an aquifer, as described in the next section.

5. Hydrogeological Implications

Most of the known in-situ bioreclamation cases have been applied to highly permeable aquifers. Contamination, however, can occur in all types of media, ranging from soils and clays to gravel and fractured rock. The tranport of nutrients to the

contaminated groundwater zones is dependent on the fluid transport and the reaction rate of the nutrient. In geologic media of low permeability the fluid velocities are very low. If the reaction rate is fast relative to the fluid velocity, the nutrient is likely to be used up by bacteria closer to the nutrient source. Under these conditions the nutrient would not be transported effectively to a large contaminated area and little or no biodegradation may take place. Biological clogging around the nutrient source is very likely to occur. If the reaction rate was slow compared to the advection of solute then it would be possible that the nutrient would be transported to the contaminated area, even in low permeability media. The ratio of advective transport and reactive transport is reflected in the dimensionless Damkoehler number which could serve as an indicator of the feasibility of a bioreclamation method in an media of certain permeability. The distance from the nutrient source to the contamination site in lower permeability media has to be reduced as much as possible. Injection well spacings should therefore be reduced and the use of subsurface drains incorporated if appropriate. Another concern in low-permeability aquifers is the reduction of permeability due to clay dispersion. Wagner et al. (1986) reports of soil conditioners which supposedly prevent clay dispersion and therefore enhance therefore transport of nutrients and bacteria.

The groundwater velocity and flow direction can be imposed in general by the arrangement of the recharge/discharge wells and their pumping rates. During bioreclamation cases, however, this imposed flow pattern is subject to changes due to permeability reductions. The addition of nutrients and oxygen source in the recharge water is responsible for permeability reductions for numerous reasons:

- If the iron or manganese content in soils or sediments is high, precipitation of iron and manganese results from oxidation in the aquifer (Smith and Tuovinen, 1985; Hackett, 1987).

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- A sediment with a high clay content can be subject to clay dispersion, and therefore to permeability reductions if leached with a sodium-rich nutrient solution

- The various injection methods for supplying oxygen to the subsurface involve the possibility that oxygen in the form of bubbles is created inducing a multi-phase flow regime. If hydrogen peroxide, for instance, transforms very rapidly, oxygen may bubble out as a separate fluid phase.

- Bacterial growth is enhanced by the addition of nutrients, and bacterial biomass might increase extensively thus reducing permeability.

Depending on the significance of the above mentioned effects, permeability reductions in biochemically active zones can alter flow velocity and flow direction significantly. Through the induced heterogeneities due to the created low permeability zones the dispersion of the contaminant might also increase. As a consequence, the prediction of groundwater flow and contaminant transport may be miscalculated if the above mentioned effects are not considered. Despite the fact that these phenomena are difficult to quantify, their consideration for successful planning of bioreclamation methods seems mandatory.

6. Literature Review

Many laboratory experiments have employed column permeameters to observe changes in hydraulic conductivity or permeability resulting from microbial activity (Allison, 1947, McCalla, 1950, Gupta and Swartzendruber, 1962, Poulovassilis, 1972, Frankenberger et al. 1979, Shaw et al., 1985). Hydraulic conductivity is a parameter used to characterize the ability of a porous medium to transmit fluids for a given hydraulic gradient. It is a volume-averaged parameter defined as the

proportionality constant in Darcy's law:

$$q = -K\frac{\partial h}{\partial s} \tag{1}$$

Where: h is the hydraulic head, $[m]$

s is the direction coordinate of flow, $[m]$

q is the specific discharge, $[m/s]$

K is the hydraulic conductivity, $[m/s]$

The hydraulic conductivity is related to the permeability k through:

$$K = \frac{k\rho g}{\mu} \tag{2}$$

Where: ρ is the fluid density, $[kg/m^3]$

μ is the fluid viscosity, $[Ns/m^2]$

g is the acceleration of gravity, $[m/s^2]$

k is the intrinsic permeability, $[m^2]$

The permeability of a porous medium is controlled by lithologic factors such as grain packing, pore shape, and specific surface, tortuosity, and connectivity (Bear, 1972). For many geologic media the permeability is also greatly affected by the degree of fracturing and cementation.

Figure 6 gives a summary of the references cited here which examine the influence of microbial growth on permeability under biotic and abiotic conditions. A perusal of the literature has shown that three types of experimental approach have been used to inhibit biological activity within the columns:

- leaching under sterile conditions (Allison, 1947; Poulovassilis, 1972; Franken-berger et al., 1979; Shaw et al., 1985).

- leaching with toxic solutions (Allison, 1947; Gupta and Swartzendruber, 1962; Shaw et al., 1985).

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References	Soil and Treatment	Solution	Hydraulic Conductivity $\frac{K_{final}}{K_{initial}}$
Allison, 1947	sterilized loam	distilled water +salts + HgCl	1
	non-sterilized loam	distilled water + salts	10^{-1}
McCalla, 1950	silty clay loam, sandy loam	tap water +0.2%succrose	1 / 10^{-1}
	uniform quartz	boiled water	1
Gupta, 1962	sand	without phenole	4×10^{-2}
	no treatment	with 0.1%phenole	1 inflow
Poulovassilis, 1972	sterile clay	distilled water	9×10^{-1}
	non sterile clay		4×10^{-2}
Frankenberger 1979	sterile	distilled water	1
	non sterile	distilled water	3×10^{-2}
		+0.05% glucose	2×10^{-3}
	silty clay loam	+0.005%KNO_3	3×10^{-3}
		0.05% glucose +0.05%KNO_3	4×10^{-4}
Shaw,1985	glass beads	distilled water	3×10^{-1}
		sterile distilled water	1
		$2 \times 10^7/ml$ Pseudomonas sp.	3×10^{-3}
		$3 \times 10^7/ml$ killed Pseudomonas sp.	0.6
		$0.1mg/ml$ SiC	5×10^{-2}
		$0.1mg/ml$ SiC + Pseudomonas sp.	1×10^{-3}

Figure 6: Literature review of laboratory experiments evaluating the influence of bacteria on the hydraulic conductivity of porous media.

- leaching under conditions with temperature slightly above freezing (McCalla, 1950; Gupta and Swartzendruber, 1962).

No changes in permeability could be observed in experiments where biological activity in the porous media was inhibited. Non-sterilized samples , however, showed a substantial decrease in hydraulic conductivity. Frankenberger et al. (1979) compared the effect of different nutrients on the hydraulic conductivity. His results show that a solution of glucose and KNO_3 was the most effective in terms of hydraulic conductivity reduction. Okubo and Matsumoto(1983), and Shaw et al.(1985), showed that the permeabilty was still more reduced when their leaching solution contained suspended solid particles.

The results of these experiments document the ability of microbial processes to reduce the permeability of a granular porous medium by as much as two or three orders of magnitude , at least for periods of reactive fluid flow on the order of hundreds of days. This is clear evidence that microbial degradation effects on the hydraulic properties ought to be taken into account in any quantitative assessment of aquifer restoration by in situ methods. One problem, however, is deciding on the means of quantifying the permeability reductions. Gupta and Swartzendruber (1962) sought a relationship between hydraulic conductivity and the total mass of microorganisms. From their experiments, changes in hydraulic conductivity were observed only above a threshold level of $4x10^6$ bacteria per gram of soil. Frankenberger et al.(1979) observed a more uniform decline in permeability with increase in bacterial mass, which they gaged with phosphatase production. Okubo and Matzumoto (1983) observed in their experiments an increase of clogging when either the substrate input concentration or the suspended particle concentration or both of them were increased. Furthermore they could show that there exist three distinct zones exhibiting different clogging rates. The first zone was identified as the aerobic

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phase and showed the fastest growth rate. The second zone was a transition zone between the aerobic and anaerobic phase, showing a slight increase in permeability. Finally a third zone, the anaerobic phase, was characterized by a continuous decrease of permeability, but at a lower rate than during aerobic growth.

It is not yet clear why or how the bacterial activity caused the permeability reduction. The following factors may all be of importance :

- mass of bacteria

- solid products produced by bacteria like exocellular polymers

- gases produced by bacteria

- disaggregation of soil grains in the porous media through bacterial consumption of aggregating organic compounds

- inorganic dissolution/precipitation reactions induced by bacteria

Considering that the threshold level of 4×10^5 bacteria per gram sand (Gupta and Swartzendruber, 1962) represents only 0.0003 % of the total volume of one gram volume of sand, bacteria mass may not be the reason for permeability reduction alone. Micrographs made by Shaw et al.(1985) show in their experiments extracellular polymers as a main cause for bacterial clogging processes. McCalla (1950) and Poulovassilis (1972) identified gas production as a major reason for permeability decreases. Other factors such as inorganic reactions (Quirk and Schofield, 1955; Suarez et al., 1984) and swelling and shrinking of clays (Goldenberg et al. , 1983; Fernandez and Quigley, 1985) may also have played a role in affecting permeability in the porous media used in the experiments.

Observations in the field suggest that bacteria are responsible for permeabilty reductions in the subsurface. Sealing effects at infiltration ponds during waste wa-

ter recharge, as well as during river infiltration were reported by Geldner (1980) and Schwarzenbach et al.(1983). Numerous examples of well clogging are also reported (Ehrlich, et al., 1973; Hijnen and van der Kooij, 1984; Smith and Tuovinen, 1985). In many cases these phenomena could be related to bacterial activity. Field groundwater samples taken by Harvey et al.(1984) in a aquifer contaminated by a sewage treatment effluent, indicated orders of magnitude higher number of bacteria within the contamination plume.

7. Laboratory Experiment

With the exception of Shaw et al.(1985) who performed their experiments with sintered glass beads, all of the above cited studies have used a porous medium composed of geologic material such as sand or loam. Because of the inherent mineralogical complexity of a geologic material it is difficult to isolate the relative importance of the numerous biological, chemical, and physical processes that could affect permeability changes. All that is known so far is that permeability reductions in shallow aquifers mainly occur as a result of bacterial activity.

Attempts to quantify these effects with respect to bacterial mass were done by Frankenberger et al.(1979). Frankenberger used a clayey loam in his experiment as the porous medium. It is doubtful, however, that Frankenberger's results can be generalized for other geological materials. The biological system of most experiments consisted of a mixed system of aerobic and anaerobic growth. Bacterial gases formed under anaerobic conditions during the denitrifying and methanogenic phase (Figure 7) might have a major impact on permeability changes.

In order to prove that permeability reductions are due mainly to bacterial gas production, Poulovassilis degassed his permeameter column under vacuum and observed a significant permeability increase. Applying a vacuum onto the perme-

Biological Gas Production			
CO_2	N_2	H_2S	CH_4
Background Concentration [mg/l]			
3	14	0	0
Gasproduction for 100 mg/l Acetate [mg/]			
20	19	26	25
Gas Dissolvable [mg/l]			
1500	18	3470	24
Gases likely to form			
	N_2		CH_4
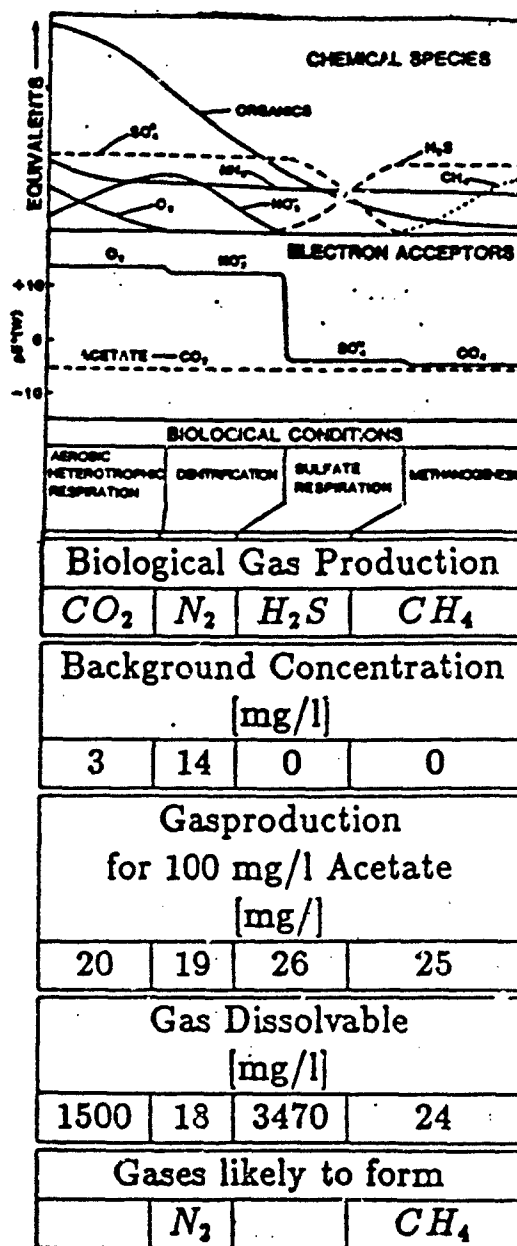
Figure 7: Possible gas production by bacteria. A microbial population is characterized by its electron acceptors. Depending on the electron acceptor present different gases can be produced by bacteria. Nitrogen and methane gas are likely to be formed under denitrifying and methanogenic conditions.

ameter, however, could have destroyed a biological matrix formed during bacterial growth which could also have exerted an influence on the permeability. It is questionable therefore to what extent the permeability increase can be ascribed to gas release, since degassing could have disturbed the porous matrix. The above workers neither offered an explanation for the hydraulic conductivity reduction, nor did they give a quantification of hydraulic conductivity reduction due to biological processes.

Objectives of Laboratory Column Experiments

A basic goal of this study was to overcome deficiencies of the earlier work cited above, so as to help evaluate the role of permeability changes in in-situ reclamation. We want to establish with our laboratory experiments a quantifiable relationship between permeability and substrate concentration. Glass beads were used as the porous medium in the experiments, to exclude all non-biological factors on permeability change, The substrate concentration and defined electron acceptor conditions are a means of controlling biomass. By maintaining a heterotrophic, aerobic biological environment, the only gas which could form due to bacterial activity is likely to be CO_2. The solubility of CO_2 under atmospheric pressure, however, is sufficiently high that gas formation would not be expected to be significant with the low substrate concentrations used in the experiments. Hence, gas evolution was excluded as a permeability reducer for the experimental conditions chosen. The permeability changes were monitored along the length of the column and over time for a constant fluid flow velocity and a given substrate input concentration. Measurements of the substrate concentration along the column as well as theoretical calculations with a biofilm model were used to help evaluate the effects of transport on substrate concentration in a flow field. The substrate distribution is related to bacterial mass by means of a biofilm model. Microscopic analysis after each experiment confirmed the

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theoretical predictions by the biofilm model concerning biomass distribution made. Hence permeability changes can be directly related to the distribution of substrate and bacterial mass within the column. Permeability distributions are compared for different substrate input concentrations.

Microscopic examination of the biomass formed can give some evidence for the cause of permeability changes. It provides some insight into the shape and size of the biomass. This may establish if the decrease in hydraulic conductivity is primarily due to volume reduction of the void space or due to the alteration of surface characteristics of the solid matrix.

Another hydraulic parameter which is addressed in our research is the hydrodynamic dispersion coefficient. Values of the dispersion coefficient measured in laboratories generally differ greatly form those evaluated in field studies (Freeze and Cherry, 1979). Dispersivity values, measured in the laboratory columns, however, could provide at least qualitative information on the influence of bacterial growth on the dispersion coefficient.

Description of Laboratory Apparatus

A fixed wall permeameter was used to measure permeability (Figure 8). A peristaltic pump provides a constant flow while manometers ports along the permeameter measure the changes in hydraulic head.

Glass beads were used as the porous material because the possibility of grain rearrangement during flow and adsorption/desorption effects are minimized. Furthermore, no shrinking or swelling as with clayey material and no mineral dissolution needs to be considered with glass beads. The organic carbon content can be controlled and the shape and surface area of the grains are well defined. A bead diameter which is close to a medium sand was chosen for the first set of experi-

Laboratory Set-Up
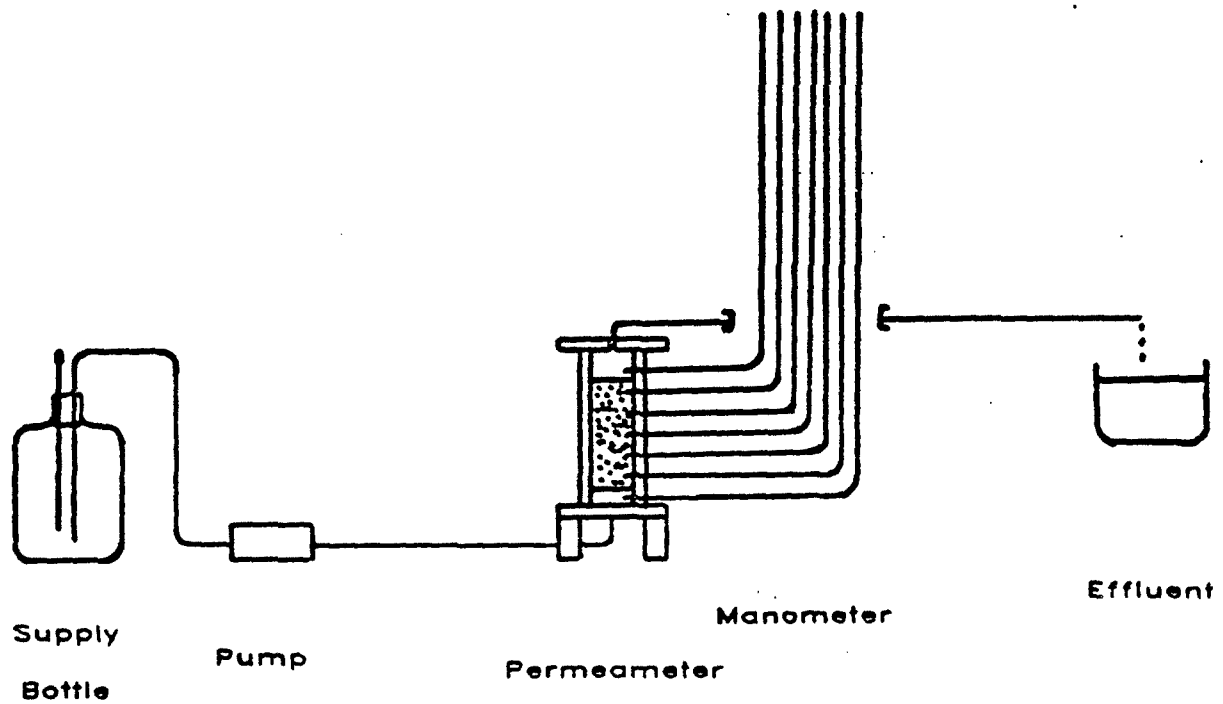
Figure 8: Laboratory apparatus for permeability experiment. Nutrients are supplied from the supply bottle through the pump to the permeameter. The permeameter was inoculated initially with a sewage-derived bacteria solution. Manometers along the permeameter track pressure differences due to permeability changes.

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ments. Glass beads of the FERRO Corporation are within a range of 0.177 and 0.210 mm. No more than 2 % are irregularly shaped and 90 % of them are true spheres. The bulk specific gravity averages close to 1.5 and the density of the solid glass is approximately 2500 kg/m^3.

A photograph of the laboratory set-up is shown in Figure 9. Plexiglass was used to fabricate the permeameters, because the experimental solution does not contain highly adsorbable organic compounds. Nylon fittings came from the Swagelok Corporation . The column length was 15 cm and its cross-sectional area was 15.55 cm^2. Manometer or lets were placed along the column. Close to the inflow they were arranged in shorter intervals, since the highest permeability reductions were expected there. The manometer fittings intrude slightly into the porous medium to avoid wall effects. The glass beads were placed on a nylon mesh with a mesh opening of 0.125 mm (Small Parts Inc.). The transparent plexiglass column was wrapped with aluminum foil to prevent growth of photosynthetic microorganisms. It was easily removed to observe possible changes of color in the porous sample due to biofilm growth. A multichannel, mini-cartridge pump (ISMATEC, Model-No. NK7624-02) maintains constant column flow. This pump can sustain a flowrate range of 8.3×10^{-10} to $4.4 \times 10^{-7} m^3/s$. Silicon is an inert material but permeable to gases, and as such it was used for the tubing from the supply bottle to the inlet of the permeameter where oxygen saturation is desired. Teflon tubing which is very inert and less permeable to oxygen was used between the permeameter outflow and sample bottle.

Experimental Procedure

The experimental procedure is outlined in Figure 10. The whole set-up was sterilized before the experiments started. The glassware was sterilized by heating
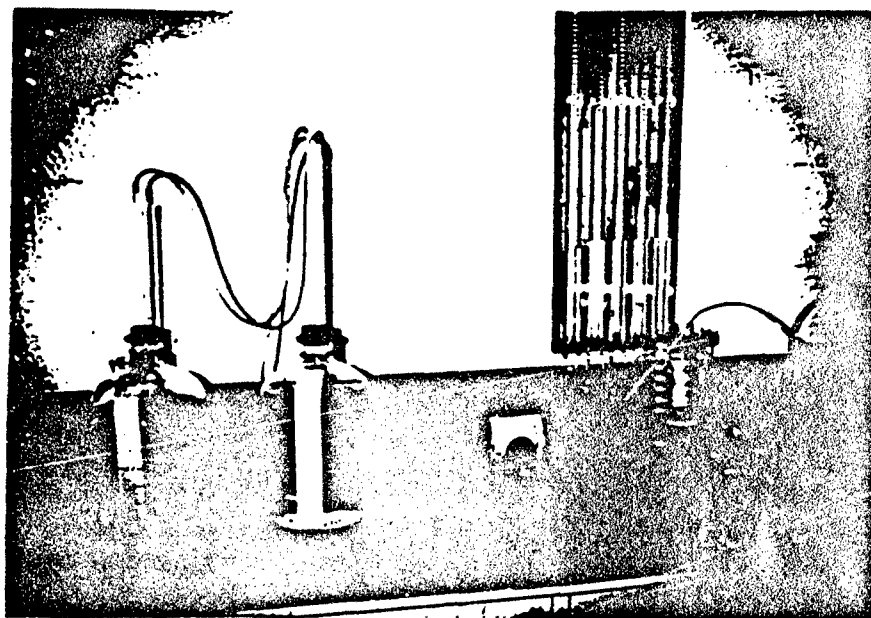
Figure 9: Photo of laboratory apparatus.
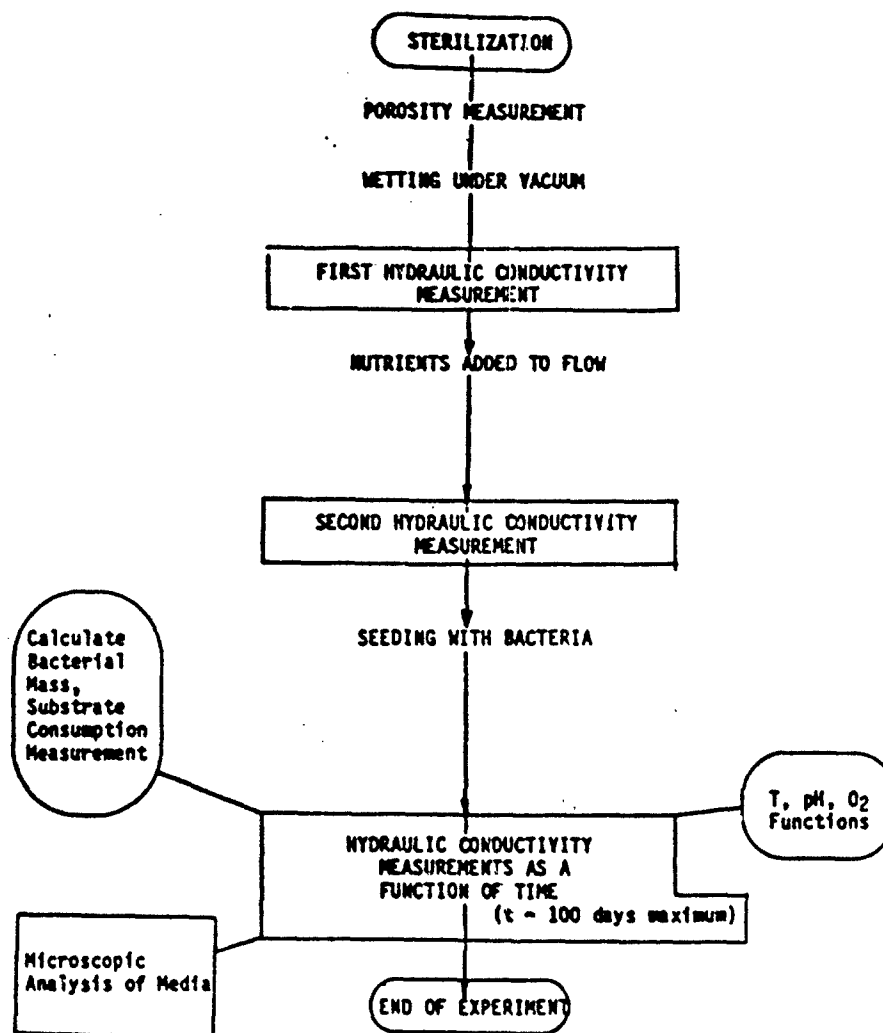
Figure 10: Flow chart of experimental procedure

in an autoclave. The plexiglass permeameter and the plastic tubing were disinfected with a 10 % chlorox solution. The column influent was prepared with distilled and sterilized water. The glass beads were poured into the column filled with water in order to avoid air inclusions. The column was closed and the virgin hydraulic conductivity measurement was madewhich served as reference value for the initial state.

A bromide ion tracer was used to provide an estimate of the hydrodynamic dispersion coefficient. The bromide breakthrough response was analyzed with an advection/dispersion transport model (Javandel et al., 1984) to evaluate the dispersion coefficient. The bromide ion was analyzed by measuring the ion concentration with an ion-chromatograph. The experimental break-through curve was fitted with an analytical solution from which the dispersion coefficient was evaluated.

A bacteria solution was prepared by diluting primary settled sewage. This solution was pumped into the column. The pumping was interrupted for six hours so that bacteria could settle in the porous medium. A phosphate buffer solution was added to the bacterial solution to prevent any cell-lysis.

After inoculation, other neccessary nutrients, such as a phosphate buffer, magnesium sulfate, calcium chloride, ferric cloride (*Standard Methods*, 1976) were added and acetate was used as the carbon source. Hydraulic conductivity measurements were taken once or twice a day in the beginning, and every second day at a later stage of the experiment. The oxygen content of the outflow and the pH was measured once a week, to ensure that the system is aerobic and that no major biological changes occurred.

One tracer test with radioactive labeled acetate as the carbon source was performed to evaluate the uptake of acetate by bacteria. One liter of nutrient solution was autoclaved and $20\mu l$ of radioactive carbon-14 ($acetic\ acid - 2 - {}^{14}C$) was added,

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so that the reactivity was at about 5000 DPM/ml (DPM = disintegrations per minute). The permeameter was leached with this solution. Samples were taken from the inflow, outflow and along the column. The reactivity of the samples indicating the percentage of uptake of the carbon source by bacteria was measured with a liquid scintillation analyzer.

At the end of the experiment a final bromide tracer test detected changes of dispersivity after bacterial growth. Samples of glass beads were taken along the column after the experiment and analyzed under a light microscope to get visual insight into volume and shape of the bacterial mass.

Experimental Results

The hydraulic conductivity was observed over time for two input concentrations of acetate: 1 mg/l and 20 mg/l (Figure 11). The hydraulic conductivity was evaluated after Darcy's law for a column length of 10 cm by measuring the hydraulic head differences at the in and outflow of the column maintaining a constant flux. There exists for both cases a lag-phase during which the hydaulic conductivity decreased very slowly or not at all, because bacterial growth had to develop before it showed a pronounced effect on hydraulic conductivity. A phase of exponential decrease of hydraulic conductivity followed the lag-phase. The hydraulic conductivity decreased about twice as fast for the higher concentration case as for the lower concentration case. After 800 hours the hydraulic conductivity seemed to change little for the lower concentration case. The observed slight fluctuations resulted probably from sloughing and replugging of biofilm mass. For the higher concentration case the hydraulic conductivity kept decreasing after 400 hours. In both cases the total hydraulic conductivity decreased significantly: in the lower concentration case by about two orders of magnitude, and in the higher concentration case by about five orders of magnitude. Almost all changes in hydraulic head occurred within the

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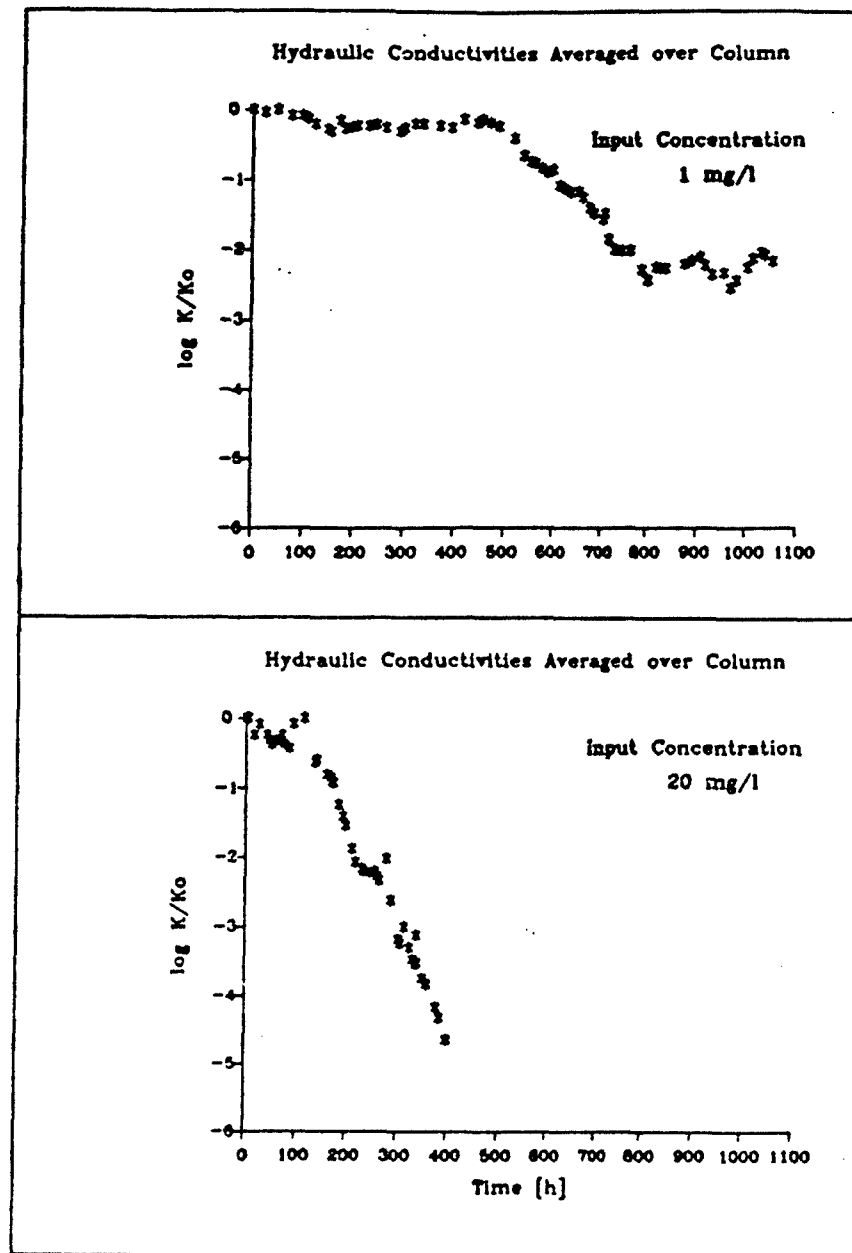
Figure 11: Hydraulic conductivities measured over time. They are average values for a column of 10 cm length, represented as the ratio of the measured hydraulic conductivity at time t to its initial value at time zero.

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first 1 cm behind the column inflow (Figure 12). In the lower concentration case, no change of hydraulic head above 1 cm was observed at all. The fact that most of the bacterial activity occurs only in the first 1 cm was confirmed by analyzing the results of the labeled acetate measurements which were taken along the column during the lower concentration experiment. It shows that 80 % of the acetate was consumed within the first 1 cm by bacteria (Figure 13).

Over the total column length, 99 % of the acetate was taken up by bacteria and transformed into biomass and carbon dioxide. The specific yield coefficient or cell yield Y which represents the ratio of mass of acetate transformed into cell mass to the mass of acetate consumed,

$$Y = \frac{grams\ of\ acetate\ transformed\ into\ cell\ mass}{grams\ of\ acetate\ consumed} \tag{3}$$

was evaluated. The difference between the mass of acetate consumed and the mass of acetate transformed into CO_2 corresponds to the mass of acetate transformed into biomass.

An average dissolved oxygen concentration of about 8 mg/l at the effluent and a constant pH of 7.1 measured during the experiment of lower input concentration showed that the biological system is governed by aerobic heterotrophic metabolism.

The dispersion coefficient seems to have increased slightly (two-fold) after bacterial growth, as shown in the results of the bromide tracer test performed before and after the higher concentration experiment (Figure 14). This increase is probably due to the heterogeneity and therefore increased tortuosity of the porous medium induced by the bacteria.

Based on these preliminary experimental results, it has become clear that future experiments should confirm the observed trends:

- a steady state hydraulic conductivity after an exponential decrease due to

Hydraulic Head Patterns
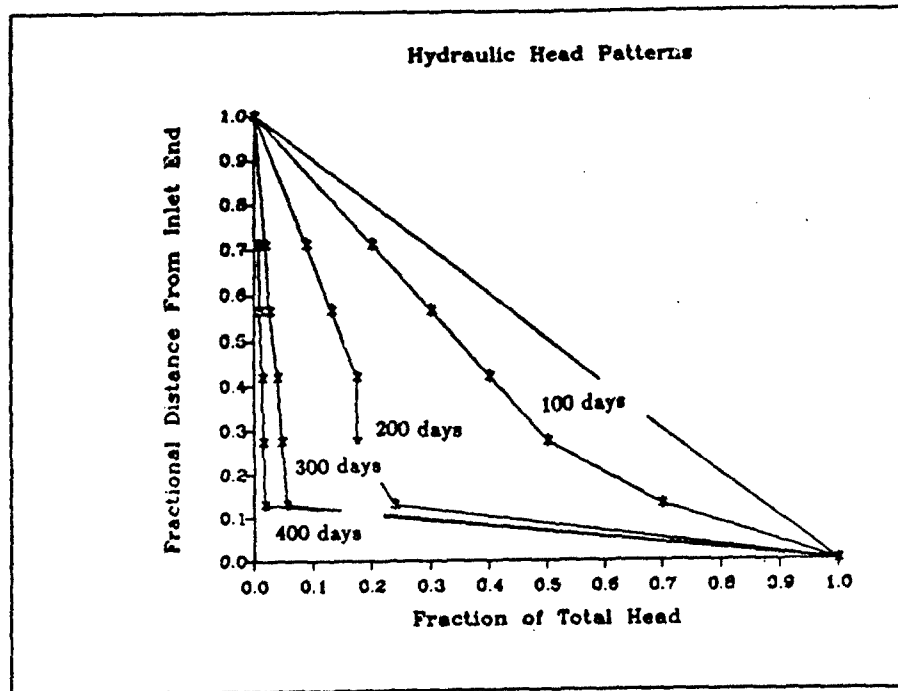
Figure 12: Hydraulic heads represented along the length of the column for different times.

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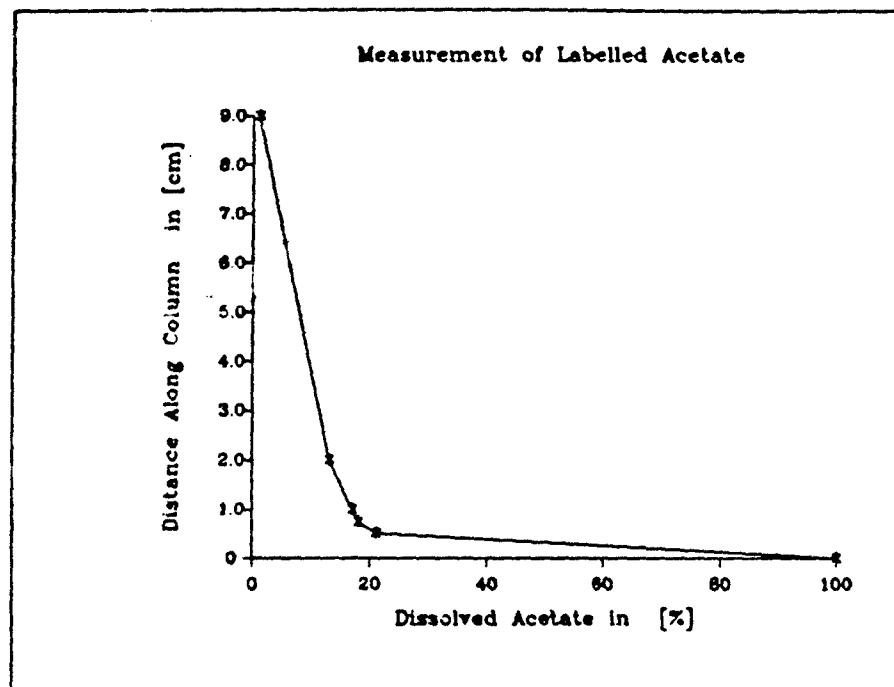
Figure 13: Concentrations of labelled acetate along the column. Concentrations of labeled acetate were measured along the column and represented as a fraction of the input concentration.
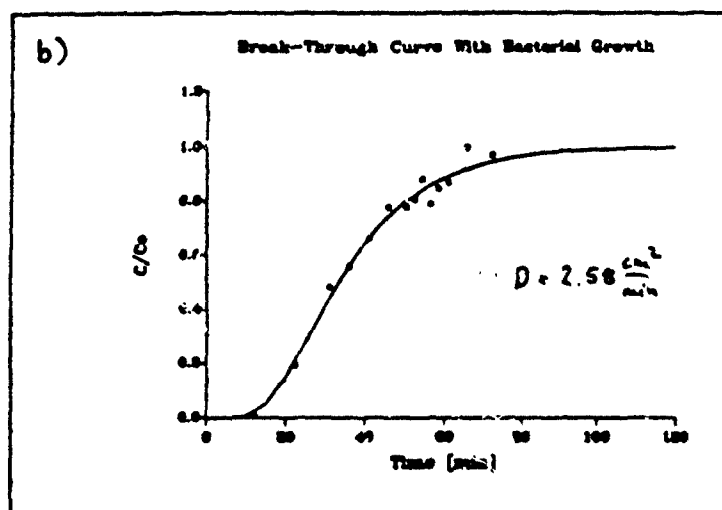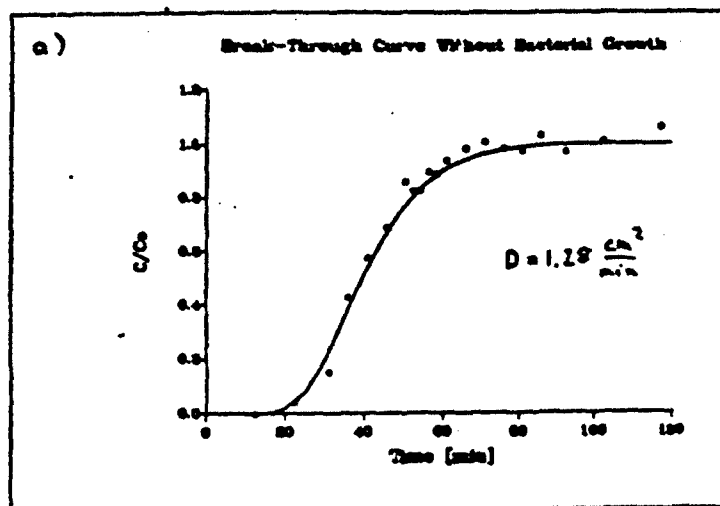
Figure 14: Breakthrough curve of a bromide tracer test. a) Breakthrough curve of a bromide tracer, measured with no bacterial growth present. b) Breakthrough curve of a bromide tracer with bacterial growth after 400 hours of leaching with a substrate concentration of 20 mg/l

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bacterial growth

- an empirical relationship between biomass expressed in terms of substrate concentration and hydraulic conductivity

- the hydraulic conductivity reduction occurs very close to the nutrient source

- an increase of dispersivity due to bacterial growth

Other factors such as varying flow rates and grain size of the porous medium may also affect the nutrient distribution and hence the biomass and hydraulic conductivity. Time did not permit the experimental evaluation of these parameters, but a theoretical analysis of the influence of these factors was performed with a biofilm model .

8. Biofilm Modeling

The mathematical biofilm model used here to simulate the experimental set-up was developed by Rittmann (1979). This model calculates substrate concentrations present at any distance and time within a column for a given input concentration . The biofilm model couples the one dimensional advection-dispersion equation with a biological reaction term. The reaction term includes transport resistance for the substrate due to turbulent flow and diffusion within the biofilm and biodegradation. The turbulent resistance and the diffusion term are both approximated by Fick's first and second law respectively. Biodegradation is expressed by a Monod term, relating substrate consumption to a reaction rate constant, bacterial mass and the half-velocity constant of the biochemical reaction:

$$\frac{\partial C}{\partial t} = -\frac{kXC}{K_s + C} \tag{4}$$

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Where: C is the substrate concentration, $[mg/l]$

k is a bacterial rate constant, $[1/s]$

X is the bacterial density, $[mg/l]$

K_c is the half velocity constant, $[mg/l]$

The model is based on the simplified assumption that bacteria attached to a surface form a biofilm of a homogeneous thickness. It is also assumed that there exists a minimum substrate concentration C_{min} below which no biofilm can be supported. A mass balance considering bacterial growth and decay allows one to calculate the biomass from the substrate concentration.

The effects of different pore sizes of porous media, different flow velocities, and different input concentrations were simulated with the model. The simulations assume a steady state situation of substrate concentration where the transport of the substrate is in equilibrium with its bacterial consumption. The results are shown in Figures 15 to 17. A different substrate input concentration affects the substrate and bacterial distribution within the column significantly. Variations in fluid velocity and grain size diameter, however, seem to have a less pronounced effect on the substrate concentration distribution. Depending on the minimum concentration C_{min} below which bacterial growth cannot be supported, the bacterial mass distribution differs greatly from the substrate concentration distribution. Further application of the model is planned to design future experiments with different input parameters.

9. Transfer of Laboratory Study to a Larger Scale

The experimental results so far evaluated apply for well-defined laboratory conditions. On a larger scale the heterogeneities and complexities of an aquifer have to be taken into account. Three factors that are important here include the average hydraulic conductivity, well clogging, and multiple electron acceptor conditions
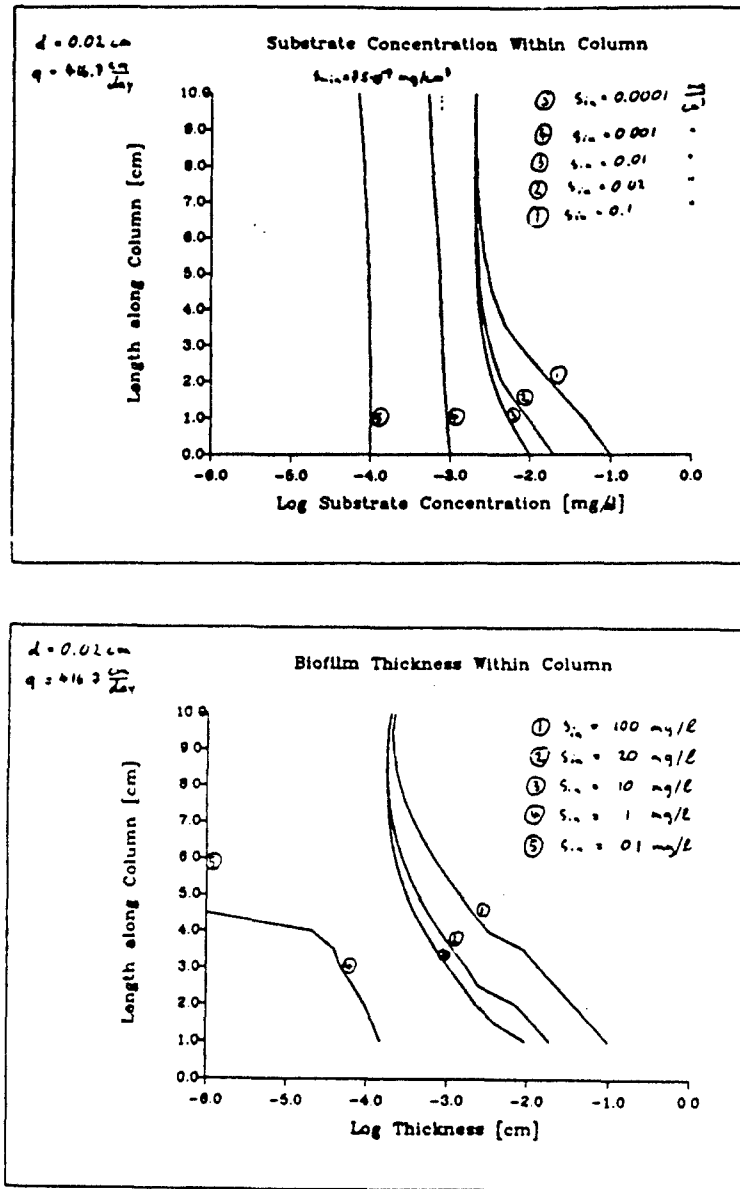
Figure 15: Biofilm simulations for different input concentrations. Substrate concentrations and biofilm thicknesses are calculated with a biofilm model for different substrate input concentrations.

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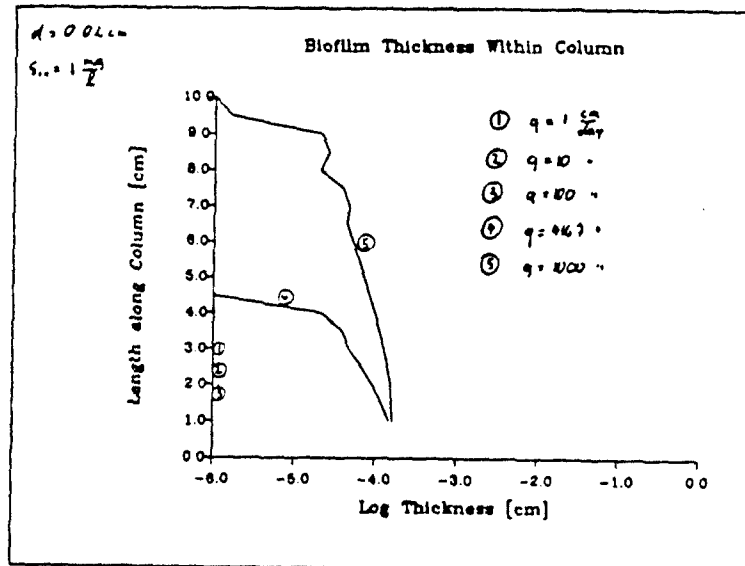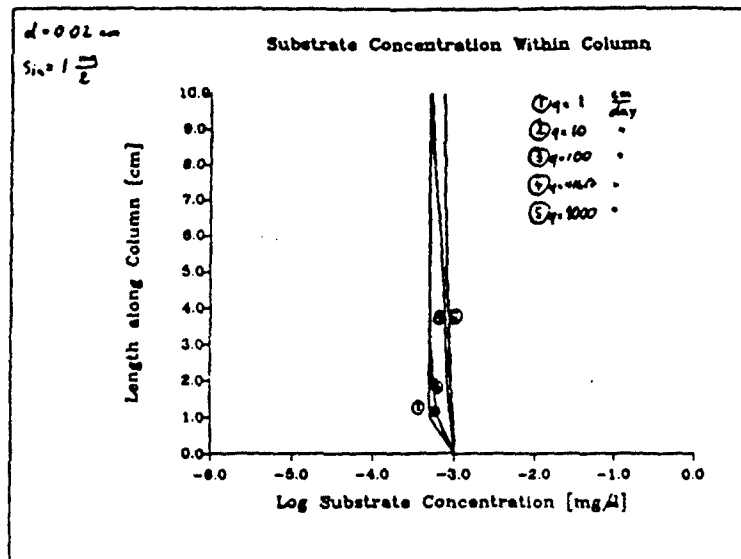
Figure 16: Biofilm simulations for different specific discharges. Substrate concentrations and biofilm thicknesses are calculated with a biofilm model for different specific discharges.
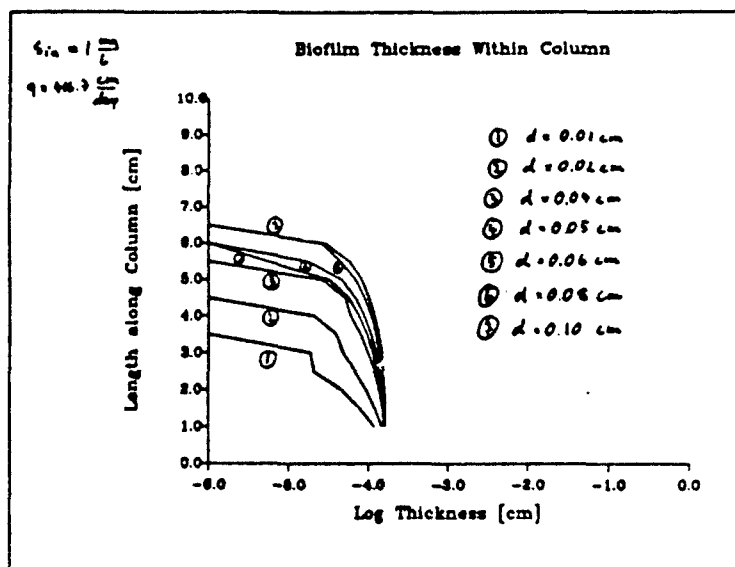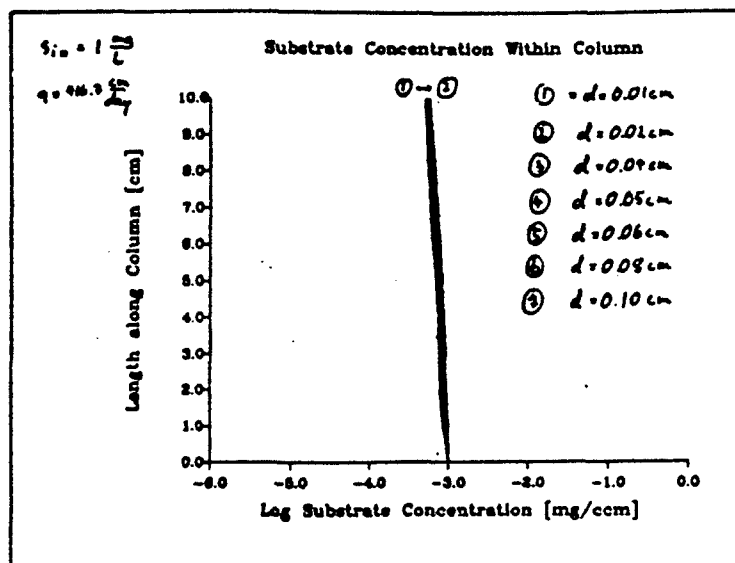
Figure 17: Biofilm simulations for different grain diameters. Substrate concentrations and biofilm thicknesses are calculated with a biofilm model for different grain diameters.

Average Hydraulic Conductivity

It can be demonstrated that a hydraulic conductivity reduction on a small scale of the order of millimeters can have a major impact on a larger scale of the order of meters. The average hydraulic conductivity of layers of different hydraulic conductivities arranged in series perpendicular to flow can be expressed by following equation(Freeze and Cherry, 1979):

$$K_{av} = \frac{d}{\sum \frac{d_i}{K_i}} \qquad (5)$$

Where: K_{av} is the averaged hydraulic conductivity, $[m/s]$

d is the total thickness of the column, $[m]$

K_i is the hydraulic conductivity for layer i, $[m/s]$

d_i is the thickness of layer i, $[m]$

In our laboratory experiment with a column of 10 cm length, the hydraulic conductivity was reduced by six orders of magnitude in the first cm above the inflow, and the hydraulic conductivity of the other 9.0 cm of the column remained unchanged. Applying equation (5) for the average hydraulic conductivity for two layers of 1 cm and 9.0 cm length respectively, one can calculate a reduction of the overall hydraulic conductivity of five orders of magnitude for the column of 10 cm length (Figure 18). The calculated and the measured values of the average hydraulic conductivity were compared for the experiment with an input concentration of 20 mg/l acetate. A hydraulic conductivity decrease by six orders of magnitude was measured in the first column segment of 1 cm length while for the total length of the column a decrease of about five orders of magnitude was observed (Figure 19). The measured hydraulic conductivity value averaged over the column length corresponds to the a calculated averaged value for two layers consisting of the first column segment and the rest of the column. If the same reasoning is applied for

Average Hydraulic Conductivities

$K_1 = 10^{-9}$

Flow Direction

$K_2 = K_3 = K_4 = 3x10^{-4}$

x = 0.1   1   10   100   m

$K_{av} = $ 10^{-9} 10^{-8} 10^{-7} 10^{-6} m/s
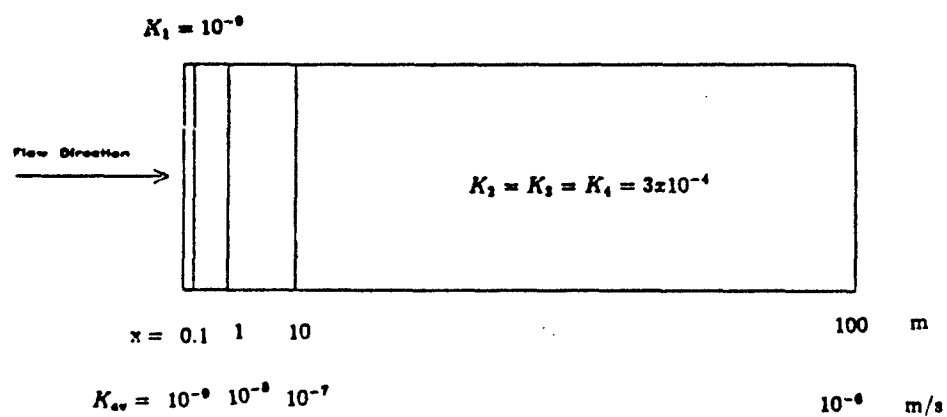
Figure 18: Average hydraulic conductivity. The average hydraulic conductivity of a large scale can be largely influenced by small scale hydraulic conductivities.
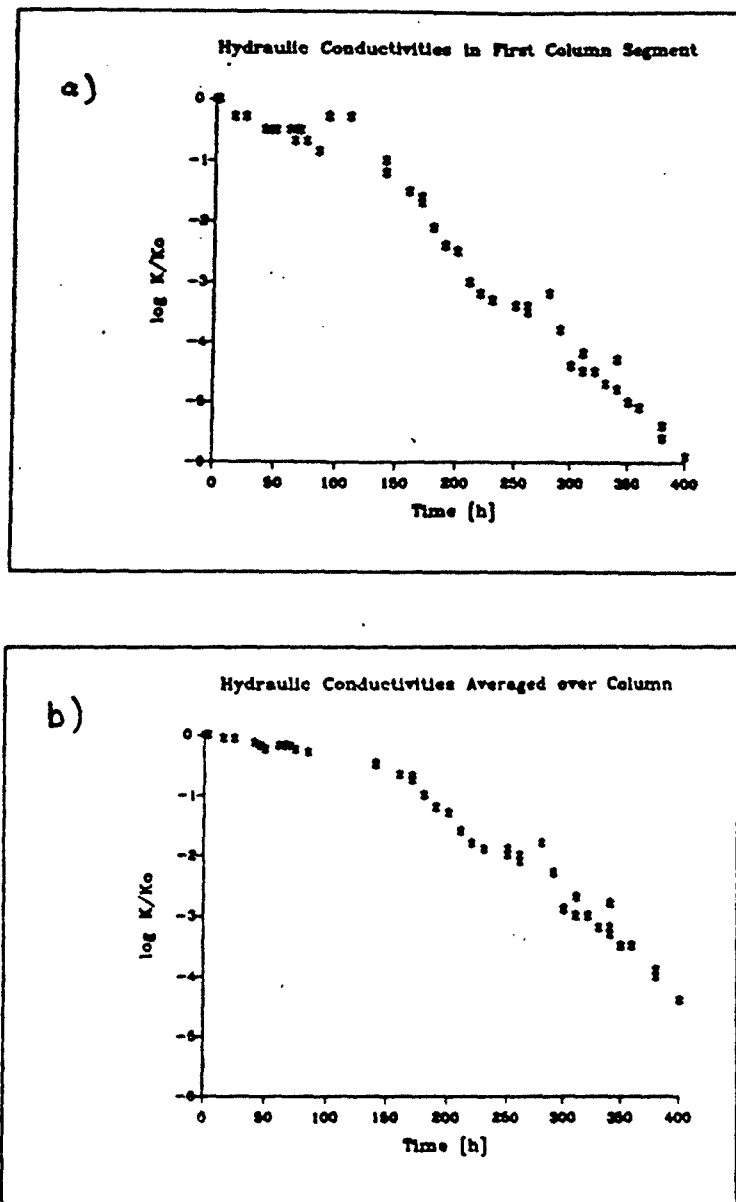
Figure 19: Hydraulic conductivities measured over time for the first column segment (a) and for the total column length (b) An input concentration 20 mg/l acetate is represented here.

columns of 1 m, 10 m, and 100 m length a hydraulic conductivity reduction of six orders of magnitude in the first cm of the column induces overall hydraulic conductivity reductions of four, three, and two orders of magnitude respectively. In other words, a reduction of hydraulic conductivity at a small scale of cm's can have a major impact on the hydraulic conductivity of a large scale of hundreds of meters.

Well Clogging

A typical biorestoration scenario will consist of several wells injecting nutrients to enhance bacterial growth (Figure 3). Well clogging is a well known phenomena (van Beek and Kooper, 1980; Oberdorfer and Peterson, 1985; Smith and Tuovinen, 1985). Since laboratory experiments showed that permeability reductions occur very close to the nutrient source it seems likely that injection wells could plug and produce only a small zone of reduced hydraulic conductivities (Figure 20a). In this case the hydraulic conductivity reductions would only have a minor effect on the fluid and contaminant transport in the aquifer. To prevent clogging it is common practice to add oxygen in form of toxic hydrogen peroxide (Yaniga and Smith, 1984) or ozone (Nagel et al., 1982) which prevents bacterial growth close to the well. In travelling through the aquifer these toxic compounds are degraded and oxygen is finally available in its non-toxic form for bacteria. A zone of lower hydraulic conductivity around the wells might form and deviate the groundwater flow around the well (Figure 20b). It is however very difficult to estimate the location and the amount of hydraulic conductivity reduction. The highly oxidizing compounds will react with the aquifer matrix. Hydraulic conductivity reduction due to mineral dissolution might overlap with the biological effects. The transport distance of the toxic compound will depend on the mineral composition of the aquifer, the reaction velocity of the compound, the advective and dispersive transport, and the

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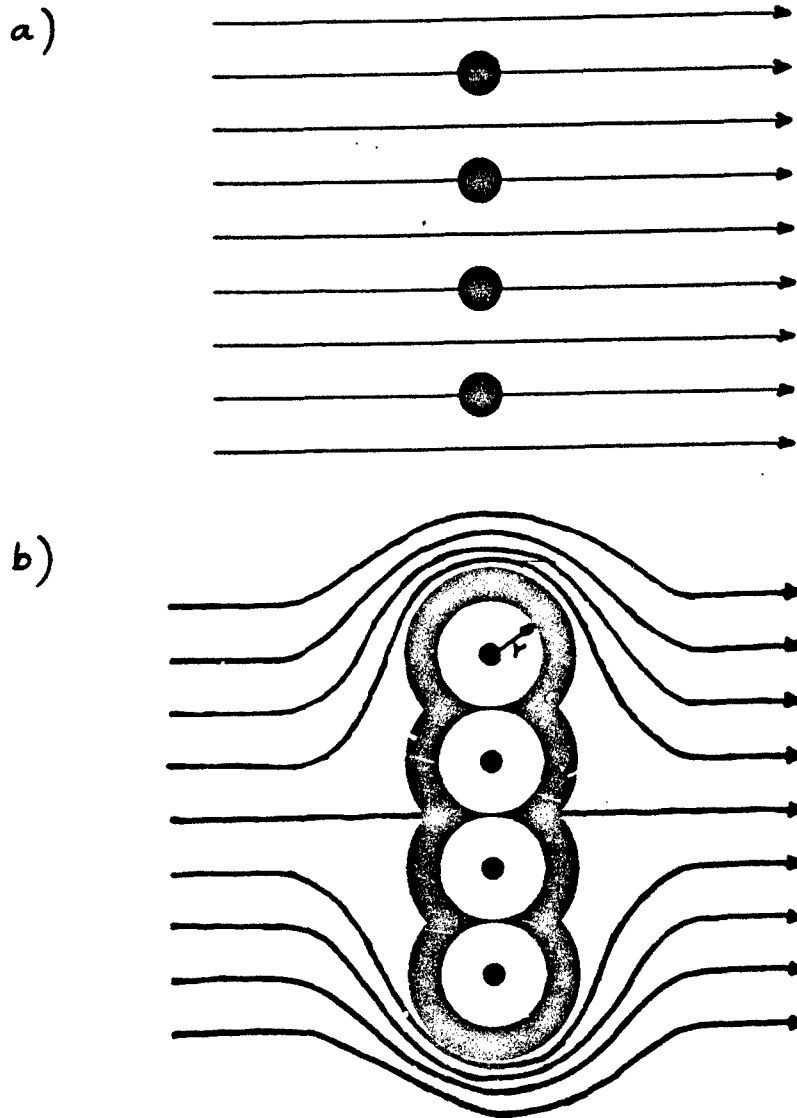
Figure 20: Possible flow patterns around injection wells. (a) Permeability reductions very close to the well does not influence the flow pattern. (b) Due to the toxicity of hydrogen peroxide bacterial growth can develop only in a distance r from the injection well. In an extreme case, high permeability reduction could deviate the polluted groundwater, preventing its degradation.

adsorption coefficient. Bacterial densities are difficult to define in the transition zone between toxic and non-toxic area. The biologically active zone might be smeared out due to diffusion and toxic activity and may therefore have a smaller effect on hydraulic conductivity, if at all.

Multiple Electron Acceptor Conditions

The above described laboratory experiments were performed under the assumptions that aerobic conditions, i.e. oxygen served as the electron acceptor, are prevailent in a large scale aquifer. On a large scale the situation might be more complex however. Depending on the background concentration and the supply of oxygen as well as the degree of bacterial activity in an aquifer, oxygen might become depleted and other compounds, such as nitrate, sulfate and carbon dioxide take over as electron acceptor (Figure 7). Thermodynamic calculations (Appendix 1) as well as observations from field experiments (Oberdorfer and Peterson, 1985) show that under denitrifying conditions (nitrate as electron acceptor) nitrogen gas and under methanogeneris (carbon dioxide as electron acceptor) methane is likely to be formed. Permeability is reported to be considerably reduced by gases (Christiansen, 1944; Gupta and Swartzendruber, 1962), so that, both, biomass and gases might contribute to significant permeability reductions. However, it is hardly possible to predict the amount and extent of gases produced as well as it is difficult to assess its relative importance for clogging effects compared to bacterial mass formation.

Summary

As pointed out at the beginning of this chapter small scale permeability reductions can have a major impact on large scale permeabilties. The situation in a large scale aquifer system is however so complex that it seems inappropriate to quantify effects of bacterial clogging in large scale aquifers at this stage of research. Despite this fact, it appears neccessary for any design of biorestoration methods

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to take into consideration permeability reductions due to bacterial activity for the following reasons:

- It is very likely that major permeability reductions due to bacteria actually occur also on a large scale.

- Permeability reductions on a large scale would alter fluid flow and therefore contaminant transport significantly. Ignoring permeability reductions could lead to erroneous predictions of fluid and contaminant transport.

- Although quantitative predictions of flow and contaminant transport are not yet possible for aquifers under the above described conditions, a qualitative analysis of the impact of permeability reductions due to bacteria should be mandatory for biorestoration design.

- A numerical model simulating fluid and contaminant transport considering biological clogging , would represent a useful tool for biorestoration design.

A first attempt at numerical modeling is described below.

10. Large Scale Modeling

Various numerical models exist that include biodegradation in the contaminant transport algorithm (Sykes, et al., 1982, Borden et al., 1984, Corapcioglu and Haridas, 1985, Benefield and Molz, 1985, Molz, 1986, Borden and Bedient, 1986). No attempt has been made so far to include hydraulic conductivity reductions due to bacterial growth in any numerical model. A numerical model was developed here to simulate fluid and contaminant transport including biodegradation and changing hydraulic conductivities due to bacterial activity (Appendix 1). The following differential equations describe the physical and biochemical system:

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The balance of mass equation for fluid flow in two dimensions at steady state considering changing hydraulic conductivities:

$$\frac{\partial}{\partial x}K(x,y,t)\frac{\partial h}{\partial x} + \frac{\partial}{\partial y}K(x,y,t)\frac{\partial h}{\partial y} = 0 \qquad (6)$$

where: $K(x,y,t)$ is the hydraulic conductivity,$[m/s]$

h is the hydraulic head, $[m]$

The balance of mass for the contaminant :

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y}) + \frac{\partial}{\partial y}(D_{xy}\frac{\partial C}{\partial x} + D_{yy}\frac{\partial C}{\partial y}) - v_x\frac{\partial C}{\partial x} - v_y\frac{\partial C}{\partial y} - kC \quad (7)$$

where: C is the contaminant concentration , $[mg/l]$

D_{ij} is the dispersion coefficient tensor, $[m^2/s]$

k is the rate constant for biodegration, $[1/s]$

v_x and v_y is the average linear velocity components, $[m/s]$

$$v_x = -\frac{K(x,y,t)}{n}\frac{\partial h}{\partial x} \qquad (8)$$

$$v_y = -\frac{K(x,y,t)}{n}\frac{\partial h}{\partial y} \qquad (9)$$

where: n is the porosity of the porous medium, $[-]$

The steady state form of (6) is based on the assumption that the hydraulic head equilibrates very quickly to changes in permeability, on a time scale much shorter than the solute transport in equation (7). The linearity of the biodegradation term is justified if dealing with relatively low concentrations. The Monod expression

$$\frac{\partial C}{\partial t} = -\frac{k'XC}{K_C + C} \tag{10}$$

where: k' is the max.spezific rate of substrate utilization, [1/s]

X is the bacterial density, [mg/l]

K_C is the Monod half velocity constant, [mg/l]

normally used to describe biodegradation, becomes approximately linear if $C > K_C$, i.e.:

$$\frac{\partial C}{\partial t} = -\frac{k'X}{K_C}C \tag{11}$$

where:

$$k = -\frac{k'X}{K_C} \tag{12}$$

Depending on the level of biological activity the hydraulic conductivities can be either constant or change over time. The following equation approximately describes the exponential decrease of hydraulic conductivity being observed in our laboratory experiments:

$$K = K_0 e^{-\lambda t} \tag{13}$$

Where: K_0 is the initial hydraulic conductivity, [m/s]

λ is a rate constant for hydraulic conductivity reduction, [1/s]

A Galerkin finite element model was developed to solve equations (6), (7), (8), (9), and (13). This model was applied to test the significance of hydraulic conductivity reductions. A fictitious aquifer was modeled including a contamination source

and an area of increased biological activity with reduced hydraulic conductivity values (Figure 21).

The contaminant leaking from its source was transported with the groundwater and eventually reached the biologically active zone. It was assumed that this zone was activated through infiltration of nutrients and that the infiltration rate was so low that it did not affect the fluid flow system in the aquifer. With infiltration the hydraulic conductivity decreased exponentially with time. One example was calculated where infiltration of nutrients was initiated 150 days after the contamination occurred. Biodegradation was not explicitly considered in this example. Comparision of the contaminant transport of both cases, with and without biological activity, show that the flow field is significantly altered (Figure 22) and the contaminant plume is retarded and dispersed after 500 days of contamination (Figure 23 and Figure 24).

Different scenarios and their effect on contaminant transport would have to be simulated in future studies because of the uncertainties in quantifying the hydraulic conductivity reductions without field data.

11. Conclusions

Bioreclamation of polluted groundwater ought to be a successfull and cost-effective treatment method. An overview of common technologies for in-situ treatment demonstrates that the success of the method will be closely linked to the hydrogeological conditions of the polluted aquifer. One purpose of this work was to demonstrate that bioreclamation schemes can be significantly affected through permeability reductions induced by bacteria. Biochemical reactions in the subsurface induced through the infiltration of nutrients for the enhancement of bacterial growth can alter hydrogeologic parameters, especially permeability. A literature

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HYDRAULIC CONDUCTIVITIES
AND FINITE ELEMENT MESH
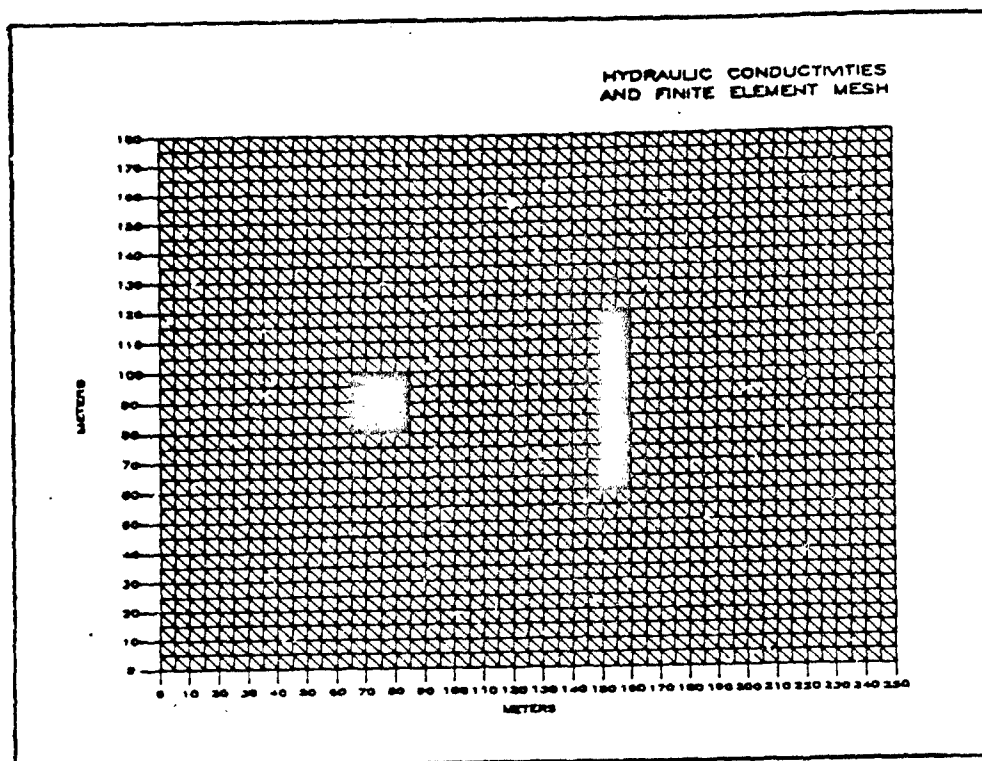
Figure 21: Finite element mesh for model aquifer with contaminant source (red)
and biodegradation area (green).

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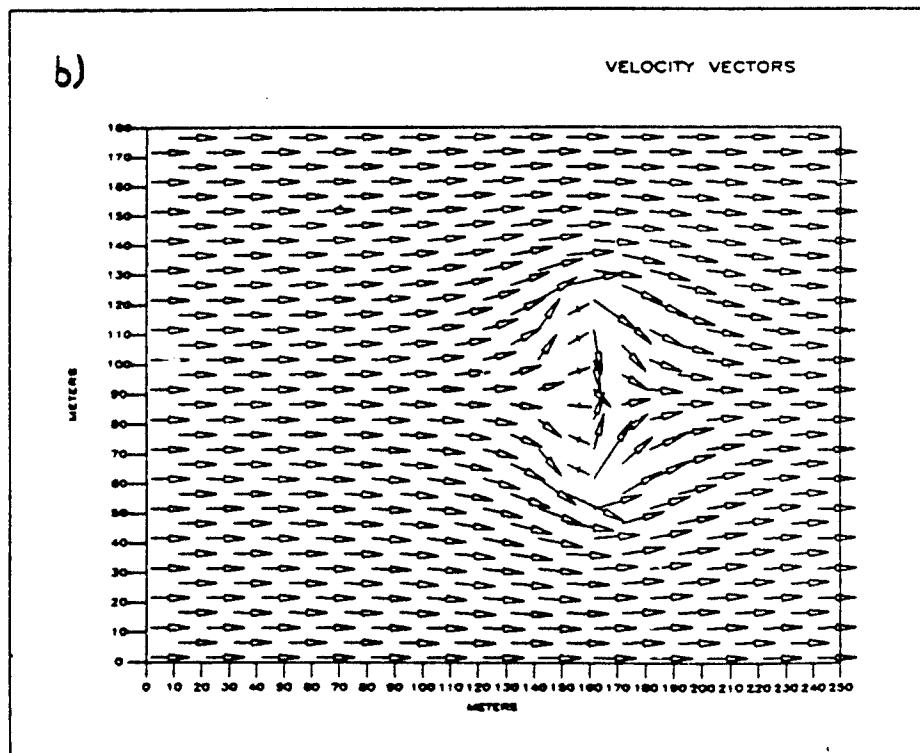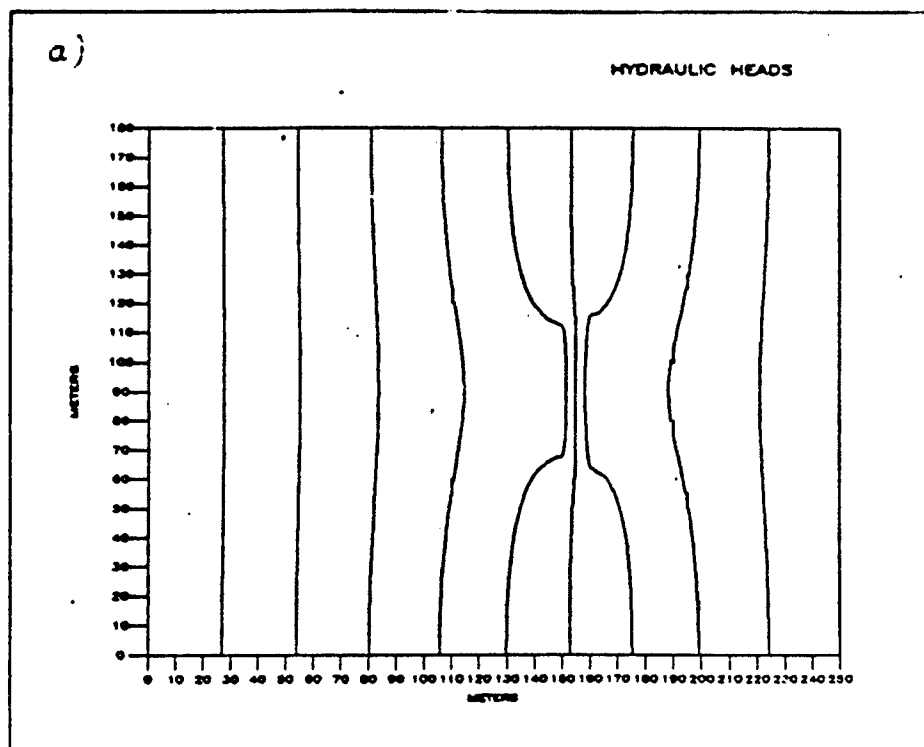
Figure 22: Numerical model results: (a) hydraulic head pattern and (b) velocity
field 500 days after contamination and 350 days after biological growth.
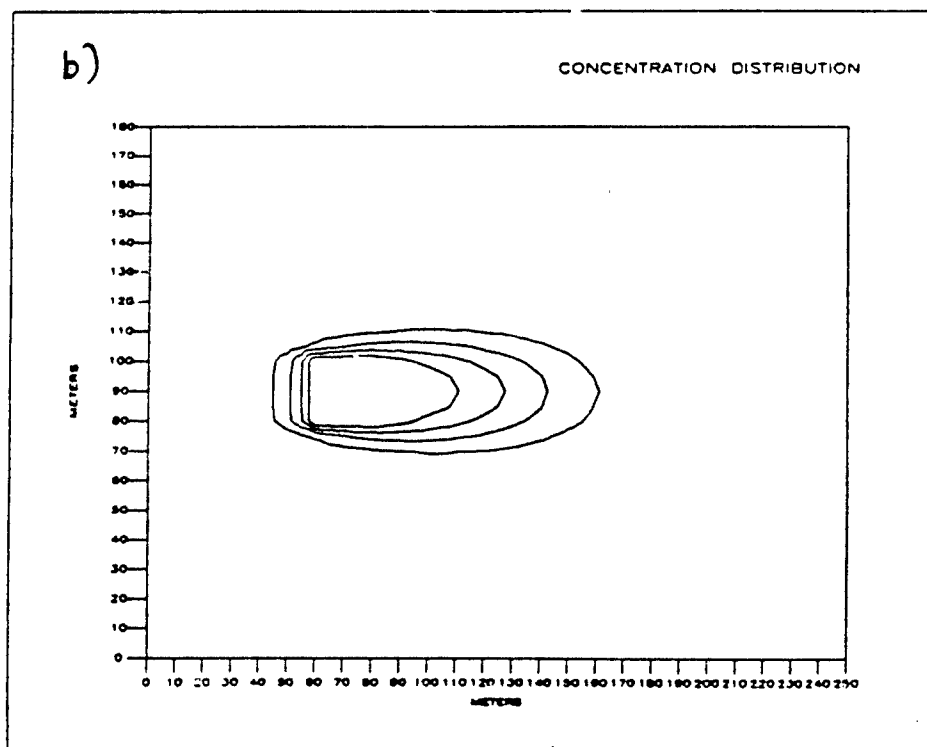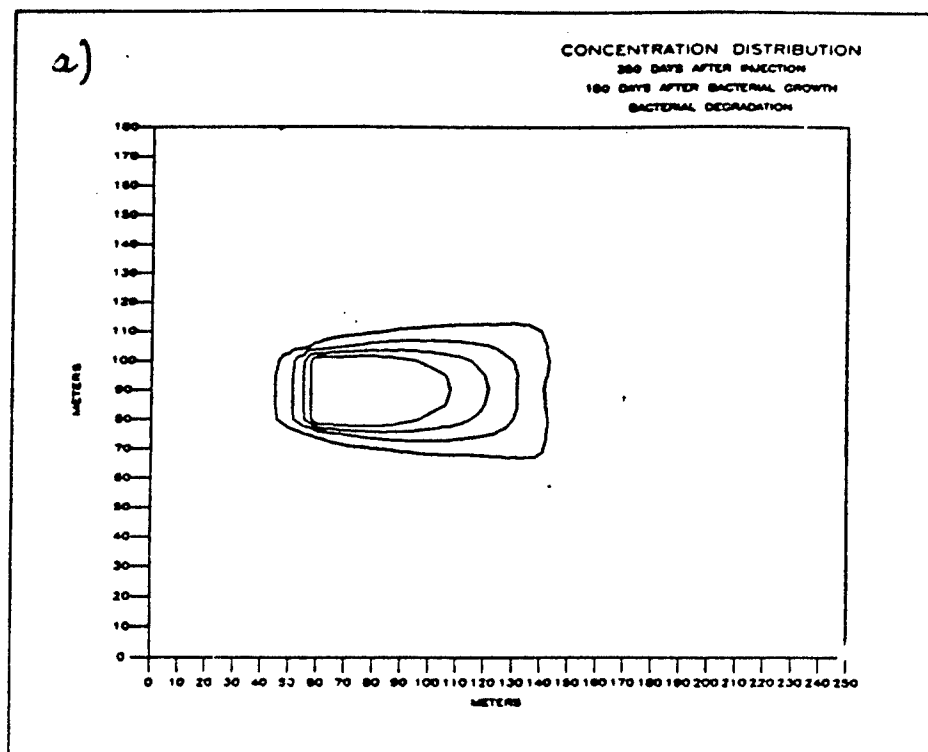
Figure 23: Spread of contamination 250 days after pollution incident: (a) with bacterial growth, (b) without bacterial growth

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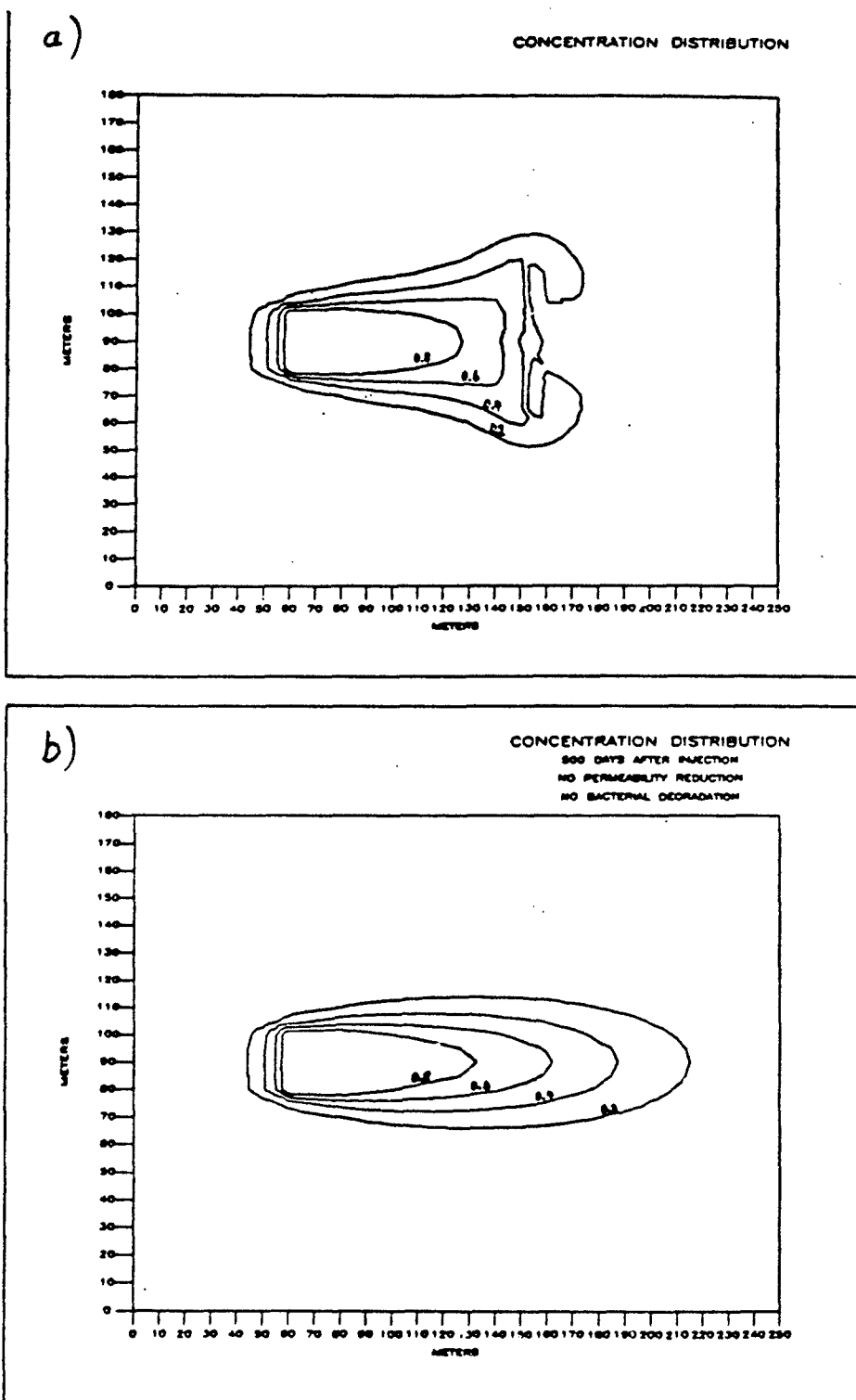
Figure 24: Spread of contamination 500 days after pollution incident: (a) with bacterial growth, (b) without bacterial growth.

review has demonstrated that permeabilities can be reduced by several orders of magnitude due to bacterial growth. In laboratory experiments we confirmed this observation. Most of the permeability changes occurred very close to the nutrient source. After a lag-phase, the permeability appeared to decrease exponentially with time. The substrate input concentration has a large influence on the degree and rate of permeability reductions. Further experiments are needed to confirm the observations made so far. The influence of other parameters, such as grain-size and fluid velocity on permeability changes need to be identified. The influence of fractures is unknown.

Difficulties are likely to be encountered in transfering the small scale results into the larger scale of an aquifer. The geological and biological systems in aquifers are generally so complex that it seems impossible at this stage of research to apply the laboratory data in the field without further assumptions. Laboratory and field tests, however, suggest that permeability reductions actually occur in the subsurface. Although quantification at this moment is not possible, a consideration of the effects of permeability reductions due to bacteria seems to be neccessary for any description of contaminant transport during biorestoration scenarios. A numerical model with the ability to test different assumptions concerning amount and extent of permeability reductions would represent a useful tool for the design of any biorestoration scheme. Field experiments could be used to validate the model for predictive purposes.

The here described research is to be considered as one step towards a better understanding for the overall hydrologic system. Further laboratory and field experiments are needed in order to fully understand the role of bacterial clogging effects on a large scale. Regardless of the scientific value of quantifying this phenomenon, the hydrogeologic effect of permeability reduction will undoubtedly play a

significant role in the practical application of in-situ biorestoration of contaminated groundwater.

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APPENDIX 1

Transport model program listing and sample input data deck

File DUA1:[WERNER.PROGRAM]CONDUC.FOR;3 (1684.2.0), last revised on 16-JUN-1987 10:34, is a 75 block sequential file owned by UIC [GGARVEN,WSIEBERT]. The records are variable length with implied (CR) carriage control. The longest record is 74 bytes.

Job CONDUC (252) queued to TXA5 on 16-JUN-1987 10:34 by user WSIEBERT, UIC [GGARVEN,WSIEBERT], under account WERNER at priority 100, started on printer _TXA5: on 16-JUN-1987 10:34 from queue TXA5.

```
WSIEBERT

CONDUC3
```

Digital Equipment Corporation - VAX/VMS Version V4.4

```
C************************************************************
C   PROGRAM CONDUC SOLVES THE GROUNDWATER FLOW EQUATION FOR STEADY STATE
C   AND TRANSIENT FLOW IN AN INHOMOGENEOUS ISOTROPIC AQUIFER
C   WITH CONSTANT HEAD AND CONSTANT FLUX BOUNDARY CONDITIONS.
C
C   PROGRAM CONDUC ALOS SOLVES THE ADVECTION DISPERSION EQUATION FOR
C   SOLUTE TRANSPORT.
C
C   CONDUC USES THE FINITE ELEMENT METHOD, TRIANGULAR ELEMENTS
C   AND LINEAR INTERPOLATION.
C
C   GAUSSIAN ELIMINATION IS USED TO THE FINITE ELEMENT EQUATIONS.
C
C   PROGRAM WAS WRITTEN BY WERNER SIEBERT, JOHNS HOPKINS UNIVERSITY,
C   JUNE 16, 1987
C
C************************************************************
C
      DIMENSION A(2000,100),B(2000),H(2000),HT(2000,6),C(2000,6),
     .    VX(4000),VY(4000),QX(4000),QY(4000),QT(4000),VBETR(4000),
     .    CONCEN(4000), KODEC(4000), IW(3),
     .    CALT(2000)
C
      COMMON/CTIME/THETAC, DCT, NTIMEC, NSTEP, TIMCON(60), NGO, TIME,
     .    TCOND
      COMMON/PARAM/COM(4000), STOR(4000), POROS(4000), DIFFUS(4000),
     .    ALPHAL(4000), ALPHAT(4000)
      COMMON/PLOT/IPE, ICOM, CONZ, CONINT, XSIZE, YSIZE, XMAX, YMAX,
     .    YMIN, DELX, DELY, IPL(250), KTAG(4000), KTAGG,
     .    ICCON, CCONZ, CCONINT
      COMMON/STEADY/BE(4000), CE(4000), AREA(4000)
C
C   CALL INPUT- AND OUTPUT-FILE
C
      CALL ASSIGN(5,'dual:[werner.program]APR.DAT')
      CALL ASSIGN(6,'dual:[werner.program]APR.AUS')
      CALL ASSIGN(7,'dual:[werner.program]APR.OUT')
C
C   CALL SUBROUTINE OPTION
C
      CALL OPTION (NTRAN, NCONC, NVEL, NTM)
C
      CALL GRID (NNODE, NELEM, NH, NV, KODA, MBAND, IBAND)
C
      CALL PLOT (NCONC, NVEL)
C
      CALL BOUND (NNODE, H, CONCEN, NCONC, NVEL)
C
      CALL PARAM (NELEM, NTRAN, NCONC, NVEL, COND, STORA, POROSI,
     .    DIFFU, ALPHL, ALPHT, MIT, TAMBDA)
C
C   OPTION OF READING IN VELOCITIES
C
      IF (NVEL.NE.1) GO TO 3
```

```
      CALL VEL (NELEM, VX, VY, VBETR)
      GO TO 1

    3 CONTINUE

      IF (NTRAN.EQ.1) GO TO 1

      CALL INIT (NNODE, HT)

    1 CONTINUE

      IF (NCONC.EQ.1) GO TO 6

      CALL INIC (NNODE,CALT)

    6 CONTINUE

      IF (NVEL.EQ.1) GO TO 4

      IF (NTM.GT.1) GO TO 14
   17 CONTINUE
      NIT=NTM
   15 CONTINUE
      NIT=NIT+1
      DO 18 M=1,NELEM
      IF (KTAG(M).EQ.1) GO TO 18
      CON(M)=CON(M)*EXP(-TAMBDA*TIME)
      IF (CON(M).LT.1.0E-10) CON(M)=1.0E-10
   18 CONTINUE
   14 CONTINUE

      CALL STEADY (NELEM, NNODE, A, B, H, NBAND, IBAND, VX, VY, VBETR,
     .                QX, QY, NCONC, IW)

      IF (NTRAN.EQ.1) GO TO 4
```

```
      CALL TRANSI (THETA, MNODE, H, DT, MTIME, NELEM,
     .             MBAND, A, HT, QX, QY, NCONC, IW)

C
C
C
    4 CONTINUE
C
C
C
      IF (NCONC.EQ.1) GO TO 2
C
C
C
      CALL CONC (NELEM, VX, VY, VBETR, IBAND,
     .           A, NNODE, C, CALT, NIT, MTN, IT, IW)
C
C
C
    2 CONTINUE
C
C
C
      IF (NIT.EQ.NTIMEC.OR.IT.EQ.NTIMEC) GO TO 7
      IF (NIT.GT.MTN) GO TO 15
      GO TO 17
C
C
C
    7 CONTINUE
C
C
C
      CALL OUTPUT (NTRAN, NVEL, NCONC, NELEM, NNODE, NTIME,
     .             H, HT, C, VX, VY)
C
C
C
      STOP
      END
C****************************************************************
C
C
C     SUBROUTINE OPTION
C
C     FORSEES DIFFERENT OPTIONS FOR THE PROGRAM
C
C****************************************************************
      SUBROUTINE OPTION(NTRAN, NCONC, NVEL, NTN)
C
C     OPTION IF STEADY STATE OR NOT: 1=STEADY STATE, 2=TRANSIENT
C
      READ(5,100) NTRAN
C
C     OPTION IF SOLUTE TRANSPORT OR NOT: 1=FLUID TRANSPORT ONLY
C                                        2=SOLUTE TRANSPORT
C
      READ(5,100) NCONC
C
```

```fortran
C     OPTION IF VELOCITIES ARE READ IN: 1=VELOCITIES READ IN
C                                        2=VELOCITIES CALCULATED
C
      READ(5,100) NVEL
C
C     OPTION IF THERE IS AN EXPONENTIAL HEYDRAULIC CONDUCTIVITY
C     DECREASE AT TIMESTEP NTH
C
      READ(5,100) NTH
C
C     FORMAT
C
  100 FORMAT(I5)
C
      RETURN
      END
C........................................................
C........................................................
C
C     SUBROUTINE GRID AFTER PROGRAM TRNSAT FROM J.F. PICKENS
C........................................................
C........................................................
C
      SUBROUTINE GRID(NNODE, NELEM,
     .               NN, NV, KODA, MBAND, IBAND)
C
C     SUBROUTINE GRID GENERATES ELEMENT INCIDENCES AND NODAL COORDINATES
C
      COMMON/NETZ/X(2000), Y(2000), IM(4000), JM(4000), KN(4000)
      DIMENSION XGRID(60), YGRID(60)
C
C     NEL:    NO. OF ELEMENTS IN X-DIRECTION IN ONE LAYER
C     NV:     NO. OF KODES IN Y-DIRECTION MINUS ONE
C     NH:     NO. OF NODES IN X-DIRECTION MINUS ONE
C     NODES NUMBERED IN OPPOSITE DIRECTION TO ELEMENT LAYERS
C     XGRID: INCREMENTAL X-SPACING OF GRID
C     YGRID: INCREMENTAL Y-SPACING OF GRID
C
C     KODA - GRID CONTROL CODE
C     KODA EQUALS 0 FOR REGULAR GRID
C     KODA EQUALS 1 IF COORDINATES ONLY TO BE READ IN
C     KODA EQUALS 2 IF COORDINATES AND INCIDENCES TO BE READ IN
C
      READ(5,100) KODA
      READ(5,600) NNODE, NELEM
      READ(5,600) NN,NV
      IF (KODA.EQ.2) GO TO 401
C
C     OPTION 0 AND 1 REQUIRE INCIDENCES OF ELEMENTS NO. 1 AND NO. 2
C     SPECIFY ELEMENT INCIDENCES FOR ELEMENTS 1 AND 2 FOR REGULAR GRID
C
      DO 10 I=1,2
      READ(5,200) IM(I), JM(I), KM(I)
   10 CONTINUE
C
      IF (KODA.EQ.1) GO TO 201
C
C     COMPUTE NODAL COORDINATES FOR REGULAR GRID
C
      READ(5,300) (XGRID(I), I=1,NH)
      READ(5,300) (YGRID(I), I=1,NV)
```

```
      M=0
      JJ=1
      MHH=MH+1
      DO 501 K=1,MHH
      IF (K.GT.1) GO TO 505
      XX=0.0D0
      GO TO 506
  505 M=M+1
      XX=XX+XGRID(M)
  506 LL=0
      MVV=MV+1
      DO 502 I=1,MVV
      IF (I.EQ.1) GO TO 503
      LL=LL+1
      Y(JJ)=Y(JJ-1)+YGRID(LL)
      GO TO 504
  503 Y(JJ)=0.0D0
  504 X(JJ)=XX
  502 JJ=JJ+1
  501 CONTINUE
  201 CONTINUE
C
C     GENERATE ELEMENTS AND INCIDENCES FOR REGULAR GRID
C
      MEL=MN*2
      IK=MEL-1
      IJ=1
      KKK=3
      DO 333 IAAA=1,2
      DO 332 IAA=1,MV
      DO 331 L=KKK,IK,2
      IM(L)=IM(L-2)+MV+1
      JM(L)=JM(L-2)+MA+1
      KM(L)=KM(L-2)+MV+1
  331 CONTINUE
      KL=IJ
      IJ=IJ+MEL
      IK=IK+MEL
      KKK=IJ+2
      KJK=MV-1
      IF (IAA.GT.KJK) GO TO 332
      IM(IJ)=IM(KL)+1
      JM(IJ)=JM(KL)+1
      KM(IJ)=KM(KL)+1
  332 CONTINUE
      KKK=4
      IJ=2
      IK=MEL
  333 CONTINUE
      IF (KODA.EQ.1) GO TO 401
      GO TO 901
  401 CONTINUE
C
C     READ COORDINATES
C
      DO 31 K=1,NNODES
      READ(5,400) X(K), Y(K)
```

```
   31 CONTINUE
      IF (KCDA.EQ.2) GO TO 500
      GO TO 901
  500 CONTINUE
C
C     READ ELEMENT INCIDENCES
C
      DO 41 I=1,MELEM
      READ(5,200) IM(I), JM(I), KM(I)
   41 CONTINUE
  901 CONTINUE
C
C     EVALUATE HALF BANDWIDTH FOR REGULAR GRID
C
      MBAND=(JM(1)-IM(1)) + 1
C
C     EVALUATE FULL BANDWIDTH FOR REGULAR GRID
C
      IBAND=2*(JM(1)-IM(1))+1
C
C     FORMATS
C
  100 FORMAT(I5)
  200 FORMAT(3I5)
  300 FORMAT(10F5.0)
  400 FORMAT(2F10.5)
  600 FORMAT(2I5)
      RETURN
      END
C••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••
C
C     SUBROUTINE PLOT
C
C     READS IN PLOT PARAMETER
C
C••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••••
      SUBROUTINE PLOT (NCONC, NVEL)
      COMMON/PLOT/IPE, ICON, CONZ, CONINT, XSIZE, YSIZE, XMAX, YMAX,
     ¹          YMIN, DELX, DELY, IPL(250), KTAG(4000), KTAGG,
     ²          ICCON, CCONS, CCONINT
C
C     READ IN PLOT PARAMETERS
C
C     IPE    = NUMBER OF NODES ON GRID BOUNDARY
C     ICON   = NUMBER OF CONTOUR LINES
C     CONZ   = MINIMUM CONTOUR VALUE
C     CONINT = CONTOUR INTERVAL
C     XSIZE  = NUMBER OF GRID POINTS IN X-DIRECTION MINUS ONE
C     YSIZE  = NUMBER OF GRID POINTS IN Y-DIRECTION MINUS ONE
C     XMAX   = ACTUAL MAXIMUM LENGTH IN X-DIRECTION
C     YMAX   = ACTUAL MAXIMUM LENGTH IN Y-DIRECTION
C     YMIN   = MINIMUM VALUE FOR Y
C     DELX   = LENGTH OF INTERVALS BETWEEN TWO NODES IN X-DIRECTION
C     DELY   = LENGTH OF INTERVALS BETWEEN TWO NODES IN Y-DIRECTION
C
      IF (NVEL.EQ.1) GO TO 1
C
      READ(5,100) IPE, ICON, CONZ, CONINT, XSIZE, YSIZE
```

```
      READ(5,200) XMAX, YMAX, YMIN, DELX, DELY

C
C     IF (NCONC.EQ.1) GO TO 2
C
C     READ IN PLOTTING PARAMETER FOR CONCENTRATION:
C     ICCON: NUMBER OF CONTOURS
C     CCONZ: LOWER BOUNDARY FOR OUTPLOT
C     CCONINT: CONCENTRATION INTERVAL
C
      READ(5,400) ICCON, CCONZ, CCONINT
      GO TO 2
C
C   1 CONTINUE
C
C
      READ(5,100) IPE, ICCON, CCONZ, CCONINT, XSIZE, YSIZE
      READ(5,200) XMAX, YMAX, YMIN, DELX, DELY
C
C     READ IN NODE NUMBERS ON BOUNDARY
C
C   2 CONTINUE
C
C
      READ(5,300) (IPL(M), M=1,IPE)
C
C     FORMATS
C
C
  100 FORMAT(2I5, 4F10.3)
  200 FORMAT(5F10.3)
  300 FORMAT(10I5)
  400 FORMAT(I5,2F10.2)
C
      RETURN
      END
C*******************************************************
C
C     SUBROUTINE BOUND
C
C     DEFINES BOUNDARY CONDITIONS LIKE CONSTANT HEAD, CONSTANT FLUX
C*******************************************************
      SUBROUTINE BOUND (NMODE, H, CONCEN, NCONC, NVEL)
      COMMON/KODE/KODEH(4000), KODEQ(4000), KODEF(4000),
     .           KODEC(4000), KODCQ(4000), KODCF(4000)
      COMMON/HRAND/Q1(4000),   Q2(4000),   Q(4000),
     .            X1(4000),   X2(4000),   Y2(4000)
      COMMON/CRAND/QC1(4000), QC2(4000), QC(4000),
     .            XC1(4000), XC2(4000), YC1(4000), YC2(4000)
      DIMENSION H(2000), CONCEN(4000)
C
C     DEFINE BOUNDARY CONDITIONS FOR FLUID FLOW
C
C     IF (NVEL.EQ.1) GO TO 8
C
```

```
C     DEFINE DIRICHLET MODES FOR FLUID FLOW
C
111   CONTINUE
      READ(5,100) J1, J2, KODEHE, HEAD
      DO 11 M=J1,J2
      KODEH(M)=KODEHE
      H(M)=HEAD
11    CONTINUE
      IF (J2.LT.MNODE) GO TO 111
C
C     DEFINE DISCHARGE AND RECHARGE MODES
C
222   CONTINUE
      READ(5,100) J1, J2, KODEQU, SINK
      DO 22 M=J1,J2
      KODEQ(M)=KODEQU
      Q(M)=SINK
22    CONTINUE
      IF (J2.LT.MNODE) GO TO 222
C
C     DEFINE MODE OF BOUNDARY FLUXES
C
333   CONTINUE
      READ(5,100) J1,J2,KODEFL,FLUX1,FLUX2,DISX1,DISY1,DISX2,DISY2
      DO 33 M=J1,J2
      KODEF(M)=KODEFL
      Q1(M)=FLUX1
      Q2(M)=FLUX2
      X1(M)=DISX1
      Y1(M)=DISY1
      X2(M)=DISX2
      Y2(M)=DISY2
33    CONTINUE
      IF (J2.LT.MNODE) GO TO 333
      IF (NCONC.EQ.1) GO TO 9
C
C     DEFINE BOUNDARY CONDITIONS FOR SOLUTE TRANSPORT
C
C     DEFINE DIRICHLET MODES FOR SOLUTE TRANSPORT
C
9     CONTINUE
444   CONTINUE
      READ(5,100) J1,J2,KODECO,CONC
      DO 44 M=J1,J2
      KODEC(M)=KODECO
      CONCEH(M)=CONC
44    CONTINUE
      IF (J2.LT.MNODE) GO TO 444
C
C     DEFINE MODES OF SOURCES AND SINKS FOR SOLUTE TRANSPORT
C
555   CONTINUE
      READ(5,100) J1, J2, KODCQU, CONSOU
      DO 55 M=J1,J2
      KODCQ(M)=KODCQU
      QC(M)=CONSOU
55    CONTINUE
      IF (J2.LT.MNODE) GO TO 555
C
```

```
C     DEFINE NODES OF BOUNDARY FLUXES FOR SOLUTE TRANSPORT
C
666   CONTINUE
      READ(5,100) J1,J2,KODCFL,FLUX1,FLUX2,FENGX1,FENGY1,FENGX2,FENGY2
      DO 66 M=J1,J2
      KODCF(M)=KODCFL
      QC1(M)=FLUX1
      QC2(M)=FLUX2
      XC1(M)=FENGX1
      YC1(M)=FENGY1
      XC2(M)=FENGX2
      YC2(M)=FENGY2
66    CONTINUE
      IF (J2.LT.MNODE) GO TO 666
C
9     CONTINUE
C
C     FORMAT
C
100   FORMAT(3I5,2F10.3,4F5.1)
200   FORMAT(F10.3)
      RETURN
      END
C*****************************************************
C
C     SUBROUTINE PARAM
C
C     READS IN AQUIFER PARAMETERS
C
C*****************************************************
      SUBROUTINE PARAM (MELEM, MTRAN, MCONC, NVEL, COND, STORA, POROSI,
     .           DIFFU, ALPHL, ALPHT, MTI, TAMBDA)
      COMMON/PARAM/COM(4000), STOR(4000), POROS(4000), DIFFUS(4000),
     .           ALPHAL(4000), ALPHAT(4000)
      COMMON/PLOT/IPE, ICOM, COMI, CONINT, XSIZE, YSIZE, XMAX, YMAX,
     .           YMIN, DELX, DELY, IPL(250), KTAG(4000), KTAGG,
     .           ICCOM, CCOMS, CCOMINT
      COMMON/CTIME/THETAC, DCT, MTIMEC, NSTEP, TIMCOM(60), NGO, TIME,
     .           TCOMD
      IF (NVEL.EQ.1) GO TO 8
C
C     READ IN HYDRAULIC CONDUCTIVITY
C
      READ(5,300) TAMBDA
3     CONTINUE
      READ(5,100) J1, J2, COND, KTAGG
      DO 10 M=J1,J2
      COM(M)=COND
      KTAG(M)=KTAGG
10    CONTINUE
      IF (J2.LT.MELEM) GO TO 3
      IF (NTRAN.EQ.1) GO TO 1
C
C     READ IN THE STORAGE COEFFICIENT
C
4     CONTINUE
      READ(5,100) J1, J2, STORA
      DO 20 M=J1,J2
```

```fortran
      STOR(M)=STORA
   20 CONTINUE
      IF (J2.LT.MELEM) GO TO 4
    1 CONTINUE
C
C     READ IN POROSITY, DIFFUSION COEFFICIENT, LONGITUDINAL DISPERSIVITY
C        TRANSVERS DISPERSIVITY
C
    5 CONTINUE
      READ(5,100) J1, J2, POROSI
      DO 30 M=J1,J2
      POROS(M)=POROSI
   30 CONTINUE
      IF (J2.LT.MELEM) GO TO 5
      IF (NCONC.EQ.1) GO TO 2
      IF (NVEL.NE.1) GO TO 6
    8 CONTINUE
      READ(5,400) J1,J2,KTAGG
      DO 35 M=J1,J2
      KTAG(M)=KTAGG
   35 CONTINUE
      IF (J2.LT.MELEM) GO TO 8
    6 CONTINUE
      READ(5,100) J1, J2, DIFFU
      DO 40 M=J1,J2
      DIFFUS(M)=DIFFU
   40 CONTINUE
      IF (J2.LT.MELEM) GO TO 6
    7 CONTINUE
      READ(5,200) J1, J2, ALPHL, ALPHT
      DO 50 M=J1,J2
      ALPHAL(M)=ALPHL
      ALPHAT(M)=ALPHT
   50 CONTINUE
      IF (J2.LT.MELEM) GO TO 7
C
C     READ IN THETA, IF IMPLICIT, EXPLICIT, OR CRANCK-NICHOLSON TIME STEP
C     READ IN TIME STEP AND NUMBER OF TIME STEPS
C     FOR CONCENTRATION CALCULATION
C
      READ(5,300) THETAC
      READ(5,300) DCT
      READ(5,200) NTIMEC, NSTEP
    2 CONTINUE
C
C     FORMAT
C
  100 FORMAT(2I5,F10.5,I5)
  200 FORMAT(2I5,2F10.5)
  300 FORMAT(F10.3)
  400 FORMAT(4I5)
      RETURN
      END
C********************************************************************
C
C     SUBROUTINE STEADY
C
C     CREATS A-MATRIX, Q-VECTOR, CALLS MATRIX SOLVER, TRANSFERS RESULTS
C
C********************************************************************
```

```fortran
      SUBROUTINE STEADY (NELEM, NNODE, A, B, N, NCONC, IBAND, VX, VY,
     ,                   VBETR, QX, QY, NCONC, IW)
      COMMON/METE/X(2000), Y(2000), IN(4000), JN(4000), KN(4000)
      COMMON/KODE/KODEH(4000), KODEQ(4000), KODEF(4000),
     ,            KODEC(4000), KODCQ(4000), KODCF(4000)
      COMMON/PARAM/CON(4000), STOR(4000), POROS(4000), DIFFUS(4000),
     ,             ALPHAL(4000), ALPHAT(4000)
      COMMON/HEAD/Q1(4000), Q2(4000), Q(4000),
     ,            X1(4000), Y1(4000), X2(4000), Y2(4000)
      COMMON/STEADY/BE(4000), CE(4000), AREA(4000)
      DIMENSION L1(4000), A(2000,100), B(2000), H(2000),
     *          L2(4000), VX(4000), VY(4000), VBETR(4000),
     *          QX(4000), QY(4000), IW(3)

C     ZERO A MATRIX
C
      DO 9 I=1,NNODE
      DO 9 J=1,IBAND
      A(I,J) = 0.0
    9 CONTINUE

C     CONDUCTANCE MATRIX
C
      DO 10 M=1,NELEM
      IEL=IN(M)
      JEL=JN(M)
      KEL=KN(M)

      BE(IEL) = Y(JEL) - Y(KEL)
      BE(JEL) = Y(KEL) - Y(IEL)
      BE(KEL) = Y(IEL) - Y(JEL)

      CE(IEL) = X(KEL) - X(JEL)
      CE(JEL) = X(IEL) - X(KEL)
      CE(KEL) = X(JEL) - X(IEL)

C     EVALUATE AREA OF ELEMENT
C
      AREA(M) = (CE(JEL)*BE(IEL) - CE(IEL)*BE(JEL))/2

C
      IW(1)=IEL
      IW(2)=JEL
      IW(3)=KEL

      DO 10 K=1,3
      I=IW(K)
      DO 10 L=1,3
      IF (IW(L).LT.I) GO TO 10
      J=IW(L)-I+1
      MZ=IW(L)

      A(I,J) = A(I,J) + (CON(M)/AREA(M)/4)
     *  *(BE(I)*BE(MZ) + CE(I)*CE(MZ))

   10 CONTINUE

C     CONDUCTANCE MATRIX AT CONSTANT HEAD BOUNDARY CONDITIONS
C     (DIRICHLET BOUNDARY CONDITIONS)
C
      DO 30 N=1,NNODE
```

```fortran
      IF (KODEH(M).NE. ) GO TO 30
      A(M,1) = (10**9)*A(M,1)
   30 CONTINUE
C
C     ZERO THE Q-VECTOR
C
      DO 35 M=1,NNODE
      Q(M)=0.0
   35 CONTINUE
C
C     EVALUATE FLUX VECTOR Q (NEUMAN BOUNDARY CONDITIONS)
C
      DO 40 M=1,NNODE
      IF (KODEF(M).NE.1) GO TO 40
      L1(M) = SQRT((X1(M)-X(M))**2 + (Y1(M)-Y(M))**2)
      L2(M) = SQRT((X2(M)-X(M))**2 + (Y2(M)-Y(M))**2)
      Q(M) = Q(M) + Q1(M)*L1(M)/2 + Q2(M)*L2(M)/2
   40 CONTINUE
C
C     FLUX VECTOR AT CONSTANT HEAD BOUNDARY CONDITIONS
C     (MIXED BOUNDARY CONDITIONS)
C
      DO 50 M=1,NNODE
      IF (KODEH(M).NE.1) GO TO 50
      Q(M) = Q(M) + A(M,1)*H(M)
   50 CONTINUE
C
C     INITIALIZE B-VECTOR
C
      DO 55 M=1,NNODE
      B(M) = 0.0
   55 CONTINUE
C
C     SOLVE LINEAR SYSTEM USING SUBROUTINE SBAND
C
      DO 60 M=1,NNODE
      B(M) = Q(M)
   60 CONTINUE
      NUMNP=NNODE
C
C     CALL SUBROUTINE SBAND
C
      CALL SBAND(A,B,NUMNP,MBAND)
C
C     TRANSFER RESULTS
C
      DO 70 M=1,NNODE
      H(M) = B(M)
   70 CONTINUE
C
C     CALCULATE THE SPECIFIC DISCHARGE
C
      DO 80 M=1,NELEM
      QX(M)=0.0
      QY(M)=0.0
      IEL=IN(M)
      JEL=JN(M)
      KEL=KN(M)
C
      BE(IEL) = Y(JEL) - Y(KEL)
```

```fortran
      BE(JEL) = Y(KEL) - Y(IEL)
      BE(KEL) = Y(IEL) - Y(JEL)
C
      CE(IEL) = X(KEL) - X(JEL)
      CE(JEL) = X(IEL) - X(KEL)
      CE(KEL) = X(JEL) - X(IEL)
C
C     EVALUATE AREA OF ELEMENT
C
      AREA(N) = (CE(JEL)*BE(IEL) - CE(IEL)*BE(JEL))/2
C
      IW(1)=IEL
      IW(2)=JEL
      IW(3)=KEL
C
      DO 85 K=1,3
      I=IW(K)
      QUX = - COM(M)*BE(I)*H(I)/AREA(M)/2
      QUY = - COM(M)*CE(I)*H(I)/AREA(M)/2
      QX(M) = QX(M) + QUX
      QY(M) = QY(M) + QUY
   85 CONTINUE
   80 CONTINUE
C
C     CALCULATE THE AVERAGE LINEAR VELOCITY
C
      DO 90 L=1,NELEM
      VX(L)=QX(L)/POROS(L)
      VY(L)=QY(L)/POROS(L)
C
C     CALCULATE THE ABSOLUTE VALUE OF THE AVERAGE LINEAR VELOCITY
C
      VAU = VX(L)**2 + VY(L)**2
      VBETR(L) = SQRT(VAU)
      IF (VBETR(L).EQ.0.0) VBETR(L)=0.000001
   90 CONTINUE
C
C     ZERO A MATRIX
C
      DO 19 I=1,NNODE
      DO 19 J=1,IBAND
      A(I,J) = 0.0
   19 CONTINUE
C
      RETURN
      END
C**********************************************************************
C
      SUBROUTINE INIT
C
C     DEFINES INITIAL CONDITIONS FOR FLUID FLOW
C
C**********************************************************************
      SUBROUTINE INIT (NMODE, HT)
      DIMENSION HT(2000,6)
C
C     DEFINE INITIAL CONDITIONS FOR SOLUTE TRANSPORT
C
  555 CONTINUE
      READ(5,200) J1, J2, HEAD
```

```
      DO 55 M=J1,J2
      HT(M,1)=HEAD
   55 CONTINUE
      IF (J2.LT.NNODE) GO TO 555
C
C
C  FORMAT
  200 FORMAT(2I5,F10.3)
      RETURN
      END
C
C********************************************************************************
C
C  SUBROUTINE TRANSI
C
C********************************************************************************
C
      SUBROUTINE TRANSI(THETA, NMODE, N,
     .                  DY, NTIME, NELEM,
     .                  MBAND, A, HT, QX, QY,
     .                  CONC, IW)
C
C
      COMMON/NETZ/X(2000), Y(2000), IN(4000), JN(4000), KN(4000)
      COMMON/KODE/KODEH(4000), KODEQ(4000), KODEF(4000),
     .            KODEC(4000), KODCQ(4000), KODCF(4000)
      COMMON/NRAND/Q1(4000), Q2(4000), Q(4000),
     .             X1(4000), Y1(4000), X2(4000), Y2(4000)
      COMMON/PARAM/CON(1000), STOR(4000), POROS(4000), DIFFUS(4000),
     .             ALPH/L(4000), ALPHAF(4000)
      COMMON/STEADY/BE(4000), CE(4000), AREA(4000)
      COMMON/TRANSI/D(2000,100), TMAL(2000,100), TMAR(2000,100)
      DIMENSION H(2000), A(2000,100),
     .          B(2000),
     .          HT(2000,6),
     .          B1(2000),
     .          L1(4000), L2(4000),
     .          QX(4000),
     .          QY(4000), IW(3)
C
C  OPTION FOR EXPLICIT, IMPLICIT OR CRANK-NICHOLSON
C
      READ(5,100) THETA
C
C  DEFINE BOUNDARY HEAD CONDITIONS
C
      DO 10 M=1,NNODE
      IF (KODEH(M).NE.1) GO TO 10
      READ(5,100) H(M)
   10 CONTINUE
C
C  DEFINE NEW BOUNDARY FLUXES
C
      DO 15 M=1,NNODE
      IF (KODEF(M).NE.1) GO TO 15
      READ(5,200) Q1(M), Q2(M)
      READ(5,300) X1(M), Y1(M), X2(M), Y2(M)
   15 CONTINUE
C
C  EVALUATE FLUX VECTOR Q
C
      DO 20 M=1,NNODE
```

```fortran
      IF (KODEF(N).NE.1) GO TO 20
      L1(N) = SQRT((X1(N)-X(N))**2 + (Y1(N)-Y(N))**2)
      L2(N) = SQRT((X2(N)-X(N))**2 + (Y2(N)-Y(N))**2)
      Q(N) = Q(N) + Q1(N)*L1(N)/2 + Q2(N)*L2(N)/2
   20 CONTINUE
C
C     READ IN TIME STEP DT
C
      READ(5,100) DT
C
C     READ IN NUMBER OF TIME STEPS
C
      READ(5,400) MTIME
C
C     ZERO A MATRIX
C
      DO 9 I=1,NNODE
      DO 9 J=1,IBAND
      A(I,J) = 0.0
    9 CONTINUE
C
C     CONDUCTANCE MATRIX
C
      DO 11 M=1,NELEM
      IEL=IM(M)
      JEL=JN(M)
      KEL=KN(M)
C
      BE(IEL) = Y(JEL) - Y(KEL)
      BE(JEL) = Y(KEL) - Y(IEL)
      BE(KEL) = Y(IEL) - Y(JEL)
C
      CE(IEL) = X(KEL) - X(JEL)
      CE(JEL) = X(IEL) - X(KEL)
      CE(KEL) = X(JEL) - X(IEL)
C
C     EVALUATE AREA OF ELEMENT
C
      AREA(M) = (CE(JEL)*BE(IEL) - CE(IEL)*BE(JEL))/2
C
      IW(1)=IEL
      IW(2)=JEL
      IW(3)=KEL
C
      DO 11 K=1,3
      I=IW(K)
      DO 11 L=1,3
      IF (IW(L).LT.I) GO TO 11
      J=IW(L)-I+1
      MZ=IW(L)
C
      A(I,J) = A(I,J) + (COM(M)/AREA(M)/4)
     *         *(BE(I)*BE(MZ) + CE(I)*CE(MZ))
C
   11 CONTINUE
C
C     EVALUATE D-MATRIX
C
      DO 25 M=1,NELEM
      IEL=IM(M)
```

```
         JEL=JN(M)
         KEL=KN(M)

C
         IW(1)=IEL
         IW(2)=JEL
         IW(3)=KEL

C
         DO 25 K=1,3
         I=IW(K)
         DO 25 L=1,3
         IF (IW(L).LT.I) GO TO 25
         J=IW(L)-I+1
         MZ=IW(L)
         IF (IW(L).EQ.IW(K)) GO TO 1
         D(I,J)=D(I,J)+STOR(M)*AREA(M)/12
         GO TO 25
    1    CONTINUE
         D(I,J)=D(I,J)+STOR(M)*AREA(M)/6
   25    CONTINUE

C
C  EVALUATE LEFT- AND RIGHT-HAND MATRIX
C
         DO 30 I=1,NNODE
         DO 30 J=1,MBAND
         TMAL(I,J) = THETA*A(I,J) + (1/DT)*D(I,J)
         TMAR(I,J) = (1-THETA)*A(I,J) - (1/DT)*D(I,J)
   30    CONTINUE

C
C  WRITE MATRIXES
C
         WRITE(6,456)
         DO 98 I=1,NNODE
         WRITE(6,987) (A(I,J),J=1,MBAND)
   98    CONTINUE
         WRITE(6,567)
         DO 87 I=1,NNODE
         WRITE(6,987) (D(I,J), J=1,MBAND)
   87    CONTINUE
         WRITE(6,678)
         DO 76 I=1,NNODE
         WRITE(6,987) (TMAL(I,J),J=1,MBAND)
   76    CONTINUE
         WRITE(6,789)
         DO 54 I=1,NNODE
         WRITE(6,987) (TMAR(I,J), J=1,MBAND)
   54    CONTINUE
  456    FORMAT(/'A-MATRIX'/)
  567    FORMAT(/'STORAGE-MATRIX'/)
  678    FORMAT(/'LEFT-HAND-SIDE-MATRIX'/)
  789    FORMAT(/'RIGHT-HAND-SIDE-MATRIX'/)
  987    FORMAT(4E10.3)

C
C  INITIAL CONDITIONS
C
         DO 35 I=1,NNODE
         HT(I,1)=H(I)
   35    CONTINUE

C
C  LOOP OVER TIME
C
```

```fortran
      DO 40 IT=1,MTIME

C     MULTIPLY MATRIX WITH VECTOR AT THE RIGHT-HAND SIDE

C     DEFINE B-VECTOR:
C     B = Q - ((1-THETA) * AM - (1/DT) * D) * HT
C     B = Q - TMAR * HT
C     B = Q - B1
C
C     DO 45 M=1,NNODE
C     B1(M) = 0.0
   45 CONTINUE

C     MULTIPLICATION OF TMAR-MATRIX WITH HT-VECTOR
C
      DO 50 I=1,NNODE
      DO 50 J=1,MBAND
      IF ((J+I-1).GT.NNODE) GO TO 2
      B1(I) = B1(I) + TMAR(I,J)*HT(J+I-1,IT)
    2 CONTINUE
      IF ((I-J).LT.1) GO TO 50
      IF ((J+1).GT.NBAND) GO TO 50
      B1(I) = B1(I) + TMAR(I-J,J+1)*HT(I-J,IT)
   50 CONTINUE

C     WRITE LEFT-HAND VECTOR
C
      DO 8888 I=1,NNODE
      WRITE(6,3333) B1(I)
 8888 CONTINUE
 3333 FORMAT (E10.3)

C     TOTAL B-VECTOR
C
C     INITIALIZE B-VECTOR
C
      DO 55 M=1,NNODE
      B(M) = 0.0
   55 CONTINUE

C     EVALUATE B-VECTOR
C
      DO 60 I=1,NNODE
      B(I) = Q(I) - B1(I)
   60 CONTINUE

C     DEFINE A-MATRIX
C
      DO 65 I=1,NNODE
      DO 65 J=1,MBAND
      A(I,J)=TMAL(I,J)
   65 CONTINUE

C     BOUNDARY CONDITIONS
C
      DO 70 M=1,NNODE
      IF (KODEH(M).NE.1) GO TO 70
      A(M,1)=(10**9)*A(M,1)
```

```fortran
          B(N)=A(N,1)*HT(N,IT)
70     CONTINUE
       NUMNP=NNODE

C
C      CALL SUBROUTINE SBAND
C
       CALL SBAND(A,B,NUMNP,MBAND)
C
C      TRANSFER RESULTS
C
       DO 75 N=1,NNODE
       HT(N,IT+1)=B(N)
75     CONTINUE
40     CONTINUE
C
C      CALCULATE THE SPECIFIC DISCHARGE FOR SOLUTE TRANSPORT MODEL
C
C
C      ASK IF SOLUTE TRANSPORT MODEL
C
       IF (NCONC.EQ.1) GO TO 3
       DO 80 IT=1,NTIME
       DO 80 M=1,NELEM
       IEL=IN(M)
       JEL=JN(M)
       KEL=KN(M)
       IW(1)=IEL
       IW(2)=JEL
       IW(3)=KEL
C
       DO 80 K=1,3
       I=IW(K)
       QX(M) = QX(M)  - CON(M)*BE(K)*HT(K,IT)/AREA(M)/2
       QY(M) = QY(M)  - .CON(M)*CE(K)*HT(K,IT)/AREA(M)/2
80     CONTINUE
3      CONTINUE
C
C      FORMAT
C
100    FORMAT(F10.3)
200    FORMAT(2F10.5)
300    FORMAT(4F10.5)
400    FORMAT(I5)
       RETURN
       END
C***************************************************************
C
C      SUBROUTINE VEL
C
C      READS IN AVERAGE LINEAR VELOCITIES FOR CONCENTRATION RUN
C
C      IF VELOCITIES WERE NOT CALCULATED IN SUBROUTINE STEADY OR TRANSI
C
C***************************************************************
       SUBROUTINE VEL (NELEM, VX, VY, VBETR)
       DIMENSION VX(4000), VY(4000), VBETR(4000)
C
1      CONTINUE
       READ(5,100) J1,J2,VVX
       DO 10 M=J1,J2
```

```
      VX(M)=VVX
   10 CONTINUE
      IF (J2.LT.MELEM) GO TO 1
    2 CONTINUE
      READ(5,100) J1,J2,VVY
      DO 12 M=J1,J2
      VY(M)=VVY
   12 CONTINUE
      IF (J2.LT.MELEM) GO TO 2
C
C
C CALCULATE THE ABSOLUTE VALUE OF THE AVERAGE LINEAR VELOCITY
C
      DO 90 L=1,MELEM
      VAU = VX(L)**2 + VY(L)**2
      VBETR(L) = SQRT(VAU)
      IF (VBETR(L).EQ.0.0) VBETR(L)=0.000001
   90 CONTINUE
C
C FORMATS
C
  100 FORMAT(2I5, F10.5)
C
C
      RETURN
      END
C*************************************************************
C
C
      SUBROUTINE IMIC
C
C DEFINES INITIAL CONDITIONS FOR FLUID FLOW AND SOLUTE TRANSPORT
C
      SUBROUTINE IMIC (NNODE, CALT)
      DIMENSION CALT(2000)
C
C DEFINE INITIAL CONDITIONS FOR SOLUTE TRANSPORT
C
  555 CONTINUE
      READ(5,200) J1, J2, CONC
      DO 55 M=J1,J2
      CALT(M)=CONC
   55 CONTINUE
      IF (J2.LT.NNODE) GO TO 555
C
C FORMAT
C
  230 FORMAT(2I5,F10.3)
      RETURN
      END
C*************************************************************
C
C SUBROUTINE CONC CALCULATES CONCENTRATION DISTRIBUTION
C
C*************************************************************
      SUBROUTINE CONC(MELEM, VX, VY, VBETR, IBAND,
     .       A, NNODE, C, CALT, NIT, NTM, IT, IW)
      COMMON/KODE/KODEH(4000), KODEQ(4000), KODEP(4000),
     .       KODEC(4000), KODCQ(4000), KODCF(4000)
```

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      COMMON/NETZ/X(2000), Y(2000), IM(4000), JM(4000), KN(4000)
      COMMON/CRAND/QC1(4000), QC2(4000), QC(4000),
     *            KC1(4000), YC1(4000), XC2(4000), YC2(4000)
      COMMON/PARAM/CON(4000), STOR(4000), POROS(4000), DIFFUS(4000),
     *            ALPHAL(4000), ALPHAT(4000)
      COMMON/STEADY/BE(4000), CE(4000), AREA(4000)
      COMMON/CONC/DISP11(4000), DISP12(4000), DISP22(4000),
     *            D(2000,100), P(2000,100),
     *            TMAL(2000,100), TMAR(2000,100)
      COMMON/CTIME/THETAC, DCT, MTIMEC, MSTEP, TIMCON(60), NGO, TIME,
     *            TCOND
      DIMENSION VX(4000), VY(4000), VBETR(4000), C(2000,6), BC1(2000),
     *            A(2000,100), B(2000), CALT(2000), IW(3)

C
C     ZERO MATRIXES
C
      DO 9 I=1,NNODE
      DO 9 J=1,IBAND
      A(I,J)=0.0
      D(I,J)=0.0
      P(I,J)=0.0
      TMAL(I,J)=0.0
      TMAR(I,J)=0.0
    9 CONTINUE
      DO 10 M=1,NELEM

C
C     CALCULATE THE LONGITUDINAL AND TRANSVERSE DISPERSIVITY COEFFICIENT
C
      DISPL = ALPHAL(M)*VBETR(M) + DIFFUS(M)
      DISPT = ALPHAT(M)*VBETR(M) + DIFFUS(M)

      DISP11(M) = ALPHAL(M)*VX(M)**2/VBETR(M) + ALPHAT(M)*VY(M)**2/
     *            VBETR(M) + DIFFUS(M)
      DISP12(M) = (ALPHAL(M) - ALPHAT(M))*VX(M)*VY(M)/VBETR(M) +
     *            DIFFUS(M)
      DISP22(M) = ALPHAL(M)*VY(M)**2/VBETR(M) + ALPHAT(M)*VX(M)**2/
     *            VBETR(M) + DIFFUS(M)

C
C     END OF THE LOOP
C
   10 CONTINUE
C
C     EVALUATE THE G--, U--, AND P-MATRIX
C
C     [G]c + [U]c + [P]dc/dt = [Q]
C
      DO 15 M=1,NELEM
      IEL=IM(M)
      JEL=JN(M)
      KEL=KN(M)

C
      BE(IEL) = Y(JEL) - Y(KEL)
      BE(JEL) = Y(KEL) - Y(IEL)
      BE(KEL) = Y(IEL) - Y(JEL)
C
      CE(IEL) = X(KEL) - X(JEL)
      CE(JEL) = X(IEL) - X(KEL)
      CE(KEL) = X(JEL) - X(IEL)
C
```

```
C     EVALUATE AREA OF ELEMENT
C
      AREA(M) = (CE(JEL)*BE(IEL) - CE(IEL)*BE(JEL))/2
C
      IW(1)=IEL
      IW(2)=JEL
      IW(3)=KEL
C
      DO 15 K=1,3
      I=IW(K)
      DO 15 L=1,3
      J=IW(L)+((IBAND+1)/2)-I
      MZ=IW(L)
C
C     G-MATRIX
C
      A(I,J)=A(I,J)+(DISP11(M)*BE(I)*BE(MZ)+DISP12(M)*(BE(MZ)*CE(I)
     . +BE(I)*CE(MZ))+DISP22(M)*CE(I)*CE(MZ))/AREA(M)/4
C
C     U-MATRIX
C
      D(I,J)=D(I,J)+(VX(M)*BE(MZ)+VY(M)*CE(MZ))/6
C
C     P-MATRIX
C
      IF (IW(L).EQ.IW(K)) GO TO 1
      P(I,J)=P(I,J)+AREA(M)/12
      GO TO 15
    1 CONTINUE
      P(I,J)=P(I,J)+AREA(M)/6
   15 CONTINUE
C
C     CREATE LEFT MATRIX
C
      DO 20 I=1,NNODE
      DO 20 J=1,IBAND
      TMAL(I,J)=THETAC*(A(I,J)+D(I,J))+P(I,J)/DCT
C
C     CREATE RIGHT MATRIX
C
      TMAR(I,J)=P(I,J)/DCT - (1-THETAC)*(A(I,J)+D(I,J))
   20 CONTINUE
C
C     ZERO A-MATRIX
C
      DO 19 I=1,NNODE
      DO 19 J=1,IBAND
      A(I,J)=0.0
   19 CONTINUE
C
C     LOOP OVER TIME
C
      IF (NIT.GE.NTN) GO TO 24
      KZAEHL=1
      KOUNT=1
      TIME=DCT
      NGO=(NTIMEC-1)/MSTEP
      IT=0
   30 CONTINUE
      IT=IT+1
```

```
   24 CONTINUE

C     MULTIPLY MATRIX WITH VECTOR AT THE RIGHT-HAND SIDE

C
C     DEFINE B-VECTOR:
C     B = QC - ((1-THETAC) *((G + U) - (1/DT) * P) * C
C     B = QC - TMAR * C
C     B = QC - BC1
C
C     WRITE OUT HYDRAULIC CONDUCTIVITIES

      WRITE(7,400) TIME, CON(385)

C     ZERO A-MATRIX
C
      DO 29 I=1,NNODE
      DO 29 J=1,IBAND
      A(I,J)=0.0
   29 CONTINUE

C
      DO 35 N=1,NNODE
      BC1(N) = 0.0
   35 CONTINUE

C
C     MULTIPLICATION OF TMAR-MATRIX WITH C-VECTOR
C
      DO 40 I=1,NNODE
      DO 40 J=1,IBAND
      KNACK=J+I-(IBAND+1)/2
      IF (KNACK.LT.1) GO TO 40
      IF (KNACK.GT.NNODE) GO TO 40
      BC1(I) = BC1(I) + TMAR(I,J)*CALT(KNACK)
   40 CONTINUE

C     TOTAL B-VECTOR
C
C     INITIALIZE B-VECTOR
C
      DO 45 N=1,NNODE
      B(I) = 0.0
   45 CONTINUE

C     EVALUATE B-VECTOR
C
      DO 50 I=1,NNODE
      B(I) = QC(I) + BC1(I)
   50 CONTINUE

C     DEFINE A-MATRIX
C
      DO 55 I=1,NNODE
      DO 55 J=1,IBAND
      A(I,J)-TMAL(I,J)
   55 CONTINUE

C     BOUNDARY CONDITIONS
C
```

```
      DO 60 M=1,NNODE
      IF (KODEC(M).NE.1) GO TO 60
      MUH=(IBAND+1)/2
      A(M,MUH)=(10.**9)*A(M,MUH)
      B(M)=A(M,MUH)*CALT(M)
   60 CONTINUE
      NUMHP=NNODE
C
C     CALL SUBROUTINE SBAND
C
      CALL ADAND(A,B,NUMHP,IBAND,IW)
C
C     TRANSFER RESULTS
C
C
C     ZERO A-MATRIX
C
      DO 39 I=1,NNODE
      DO 39 J=1,IBAND
      A(I,J)=0.0
   39 CONTINUE
C
      DO 65 M=1,NNODE
      CALT(M)=B(M)
   65 CONTINUE
C
      IF (KRAKNL.NE.NSTEP) GO TO 70
      DO 75 M=1,NNODE
      TIMCOM(KOUNT)=TIME
      C(M,KOUNT)=B(M)
   75 CONTINUE
      KRAKNL=1
      TIME=TIME+DCT
      KOUNT=KOUNT+1
      IF (IT.EQ.NTIMEC) GO TO 26
      IF (IT.GE.NTN.OR.NIT.GE.NTN) GO TO 26
      GO TO 30
   70 CONTINUE
      KRAKNL=KRAKNL+1
      TIME=TIME+DCT
      IF (IT.EQ.NTIMEC) GO TO 26
      IF (IT.GE.NTN.OR.NIT.GE.NTN) GO TO 26
      GO TO 30
   26 CONTINUE
C
C     FORMAT
C
  100 FORMAT(F10.5)
  200 FORMAT(I5)
  300 FORMAT(2I5,F10.5)
  400 FORMAT(F10.2, F10.6)
C
      RETURN
      END
C***********************************************
C
C     SUBROUTINE OUTPUT
C
```

```
C     WRITES OUT RESULTS
C
C***********************************************************
      SUBROUTINE OUTPUT (NTRAN, NVEL, NCONC, NELEM, NNODE, NTIME,
     *                   H, HT, C, VX, VY)

      DIMENSION H(2000), HT(2000,6), C(2000,6), VX(4000), VY(4000)
      COMMON/PLOT/IPE, ICON, CONZ, CONINT, XSIZE, YSIZE, XMAX, YMAX,
     *            YMIN, DELX, DELY, IPL(250), KTAG(4000), KTAGG,
     *            ICCON, CCONZ, CCCNINT
      COMMON/NETZ/X(2000), Y(2000), IN(4000), JN(4000), KN(4000)
      COMMON/CTIME/THETAC, DCT, NTIMEC, NSTEP, TIMCON(60), NGO, TIME,
     *             TCOND

C
C     WRITE OPTIONS
C
      WRITE(6,300) NVEL, NCONC, NTRAN, NTIME, NTIMEC, NGO
      WRITE(6,300) NELEM
      WRITE(6,300) NNODE

C
C     WRITE PLOTTING PARAMETERS COMMON FOR ALL CASES
C
      WRITE(6,200) XMAX, YMAX, YMIN, DELX, DELY
      WRITE(6,300) IPE
      WRITE(6,300) (IPL(M), M=1,IPE)
      WRITE(6,300) (IN(M), M=1,NELEM)
      WRITE(6,300) (JN(M), M=1,NELEM)
      WRITE(6,300) (KN(M), M=1,NELEM)
      WRITE(6,500) (X(M), M=1,NNODE)
      WRITE(6,500) (Y(M), M=1,NNODE)

C
C     WRITE THE TAGS FOR DIFFERENT HYDRAULIC CONDUCTIVITIES
C
      WRITE(6,300) (KTAG(M), M=1,NELEM)
      WRITE(6,700) (VX(M), M=1,NELEM)
      WRITE(6,700) (VY(M), M=1,NELEM)

C
C     WRITE PLOTTING PARAMETERS FOR FLUID FLOW CALCULATION
C
      IF (NVEL.EQ.1) GO TO 1
      WRITE(6,100) IPE, ICON, CONZ, CONINT, XSIZE, YSIZE
      IF (NTRAN.NE.1) GO TO 2
      WRITE(6,500) (H(M), M=1,NNODE)
      GO TO 3
    2 CONTINUE
      DO 10 IT=1,NTIME,20
      WRITE(6,100) IT
      DO 20 M=1,NNODE
      IF (HT(M,IT).LT.0.0) HT(M,IT)=0.0
   20 CONTINUE
      WRITE(6,800) (HT(M,IT), M=1,NNODE)
   10 CONTINUE

C
C     WRITE PLOTTING PARAMETERS FOR FLUID AND SOLUTE TRANSPORT
C
    3 CONTINUE
      IF (NCONC.EQ.1) GO TO 4
      WRITE(6,900) ICCON, CCONZ, CCONINT
      GO TO 5

C
C     WRITE PLOTTING PARAMETERS FOR SOLUTE TRANSPORT ONLY
```

```
C
   1 CONTINUE
     WRITE(6,100) IPE, ICCOM, CCOM2, CCOMNT, XSIZE, YSIZE
C
C  SET NEGATIVE CONCENTRATIONS TO ZERO
C
   5 CONTINUE
     DO 30 KOUNT=1,NGO
     WRITE(6,500) TIMCOM(KOUNT)
     DO 40 M=1,MNODE
     IF (C(M,KOUNT).LT.0.0) C(M,KOUNT)=0.0
  40 CONTINUE
     WRITE(6,800) (C(M,KOUNT), M=1,MNODE)
  30 CONTINUE
   4 CONTINUE
C
C  FORMAT
C
 100 FORMAT(2I5,4F10.2)
 200 FORMAT(5F10.2)
 300 FORMAT(10I5)
 500 FORMAT(5F10.3)
 600 FORMAT(I5,5X,I5,5X,F10.5)
 700 FORMAT(5F10.3)
 800 FORMAT(10F8.2)
 900 FORMAT(I5,2F10.2)
     RETURN
     END
C*************************************************************
C
C  SUBROUTINE SBAND
C
C  GAUSSIAN ELIMINATION FOR A SYMMETRIC, POSITIVE DEFINITE BAND MATRIX
C
C*************************************************************
     SUBROUTINE SBAND(A,B,NUMNP,MBAND)
     REAL*8 NUO,NU,MUL
     DIMENSION A(2000,100), B(2000)
C
C  TRIANGULARIZATION
C
     DO 30 N=1,NUMNP
     DO 20 L=2,MBAND
     IF (A(N,L).EQ.0.0) GO TO 20
     C=A(N,L)/A(N,1)
     I=N+L-1
     IF (I.GT.NUMNP) GO TO 20
     J=0
     DO 10 K=L,MBAND
     J=J+1
  10 IF(A(N,K).NE.0.0) A(I,J)=A(I,J)-C*A(N,K)
     A(N,L)=C
     B(I)=B(I)-A(N,L)*B(N)
  20 CONTINUE
     B(N)=B(N)/A(N,1)
  30 CONTINUE
C
C  BACK SUBSTITUTION
C
     N=NUMNP
```

```fortran
   40 DO 50 K=2,MBAND
      L=M+K-1
      IF (L.GT.NUMNP) GO TO 60
      IF (A(M,K).NE.0.0) B(M) = B(M)-A(M,K)*B(L)
   50 CONTINUE
   60 M=M-1
      IF (M.GT.0) GO TO 40
      RETURN
      END
C.....................................................................
C
C
C
C SUBROUTINE ABAND PERFORMS GAUSSIAN ELIMINATION FOR NON-SYMMETRIC
C                  BANDMATRICES (DIAGONALLY DOMINANT)
C.....................................................................
C
      SUBROUTINE ABAND(A,B,NUMNP,IBAND,IW)
C
      REAL*8 MUO,MU,MUL
C
      DIMENSION A(2000,100),B(2000),IW(3)
      IJ=(IBAND-3)/2
      IJ2=IJ+2
      IJ3=IJ+3
C
C TRIANGULARIZATION
C
      DO 30 M=1,NUMNP
      IF(A(M,IJ2).GT.1.3D-10)GOTO 5
      WRITE(6,7)M
    7 FORMAT(4X,'DIVIDED BY ZERO AT NODE',I4)
      STOP
    5 B(M)=B(M)/A(M,IJ2)
      IF(M.GE.NUMNP)GO TO 30
      K=0
   10 DO 25 J=IJ3,IBAND
      K=K+1
      A(M,J)=A(M,J)/A(M,IJ2)
      KK=0
      DO 20 I=IJ3,IBAND
      KK=KK+1
      L=M+I-IJ2
      IF(L.GT.NUMNP)GO TO 20
      M=IJ2+K-KK
      MM=IJ2-KK
      A(L,M)=A(L,M)-A(L,MM)*A(M,J)
   20 CONTINUE
      JJ=IJ2-K
      LL=M+J-IJ2
      IF(LL.GT.NUMNP)GO TO 30
      B(LL)=B(LL)-A(LL,JJ)*B(M)
   25 CONTINUE
   30 CONTINUE
C
C BACK SUBSTITUTION
C
      M=NUMNP
   40 M=M-1
      IF(M.LE.0)RETURN
      DO 50 J=IJ3,IBAND
      L=M+J-IJ2
```

```
   IF(L.GT.NUMMP)GO TO 50
   B(M)=B(M)-A(M,J)*B(L)
50 CONTINUE
   GO TO 40
   END
```

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Digital Equipment Corporation - VAX/VMS Version V4.4

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0.0	5.0	0.0	5.0	0.000	0.000	1 0	443	444
0.0	5.0	0.0	5.0	0.000	0.000	1 0	445	461
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0.0	5.0	0.0	5.0	0.000	0.000	1 0	517	518
0.0	5.0	0.0	5.0	0.000	0.000	1 0	519	520
0.0	5.0	0.0	5.0	0.000	0.000	1 0	554	555
0.0	5.0	0.0	5.0	0.000	0.000	1 0	556	557
0.0	5.0	0.0	5.0	0.000	0.000	1 0	591	592
0.0	5.0	0.0	5.0	0.000	0.000	1 0	593	594
0.0	5.0	0.0	5.0	0.000	0.000	1 0	628	629
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0.0	5.0	0.0	5.0	0.000	0.000	1 0	852	853
0.0	5.0	0.0	5.0	0.000	0.000	1 0	867	888
0.0	5.0	0.0	5.0	0.000	0.000	1 0	924	925
0.0	5.0	0.0	5.0	0.000	0.000	1 0	926	927
0.0	5.0	0.0	5.0	0.000	0.000	1 0	961	964
0.0	5.0	0.0	5.0	0.000	0.000	1 0	963	999
0.0	5.0	0.0	5.0	0.000	0.000	1 0	928	1000
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0.0	5.0	0.0	5.0	0.000	0.000	1 0	1035	1038
0.0	5.0	0.0	5.0	0.000	0.000	1 0	1037	1073
0.0	5.0	0.0	5.0	0.000	0.000	1 0	1074	1075
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   1    3600
        -0.500
        10.000

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461     465
466     497
498     502
503     534
535     539
540     571
572     576
577     608
609     613
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